

Scattering Models for Ultracold Atoms

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Abstract

We present a review of scattering models that can be used to describe the low-energy behavior of identical bosonic atoms. In the simplest models, the only degrees of freedom are atoms in the same spin state. More elaborate models have other degrees of freedom, such as atoms in other spin states or diatomic molecules. The parameters of the scattering models are specified by giving the S-wave phase shifts for scattering of atoms in the spin state of primary interest. The models are formulated as local quantum field theories and the renormalization of their coupling constants is determined. Some of the parameters can be constrained by renormalizability or by the absence of negative-norm states. The Green's functions that describe the evolution of 2-atom states are determined analytically. They are used to determine the T-matrix elements for atom-atom scattering and the binding energies of diatomic molecules. The scattering models all exhibit universal behavior as the scattering length in a specific spin state becomes large.

1 Introduction

The development of methods for trapping atoms and cooling them to ultralow temperatures has launched the new field of *cold atom physics*. Among the dramatic achievements in this field have been the creation of *Bose-Einstein condensates* of bosonic atoms and *superfluids* of fermionic atoms. At the low temperatures at which these phenomena occur, the de Broglie wavelengths of the atoms are much larger than their sizes or the ranges of their interactions. This makes the behavior of the atoms insensitive to many of the details of atomic structure and interatomic interactions. The atoms can be treated as

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point particles and their interactions can be described very accurately by simple models.

One class of models that is particularly convenient for describing ultracold atoms is *scattering models*. Scattering models are formulated in terms of parameters that describe the low-energy scattering of atoms. The simplest example is the *Zero-Range Model* whose only interaction parameter in the 2-body sector is the *S-wave scattering length*. The scattering length is the most important interaction parameter governing the behavior of cold atoms. The primary advantage of scattering models for describing cold atoms is that their parameters are directly related to physical observables at the relevant energy scale.

Another advantage of scattering models is that there are many useful models that can be solved analytically in the 2-body sector. There are very few analytic results on the 3-body and higher n -body problem, but having an analytic solution to the 2-body problem is a great simplification in the numerical solution of higher few-body problems. The analytic solution of the 2-body problem is also useful in the many-body problem, because interaction effects in low-density systems of atoms are dominated by 2-body interactions.

A particularly convenient class of scattering models is ones with *local interactions*. In these models, atoms interact with each other only when they are at the same point in space. Such a simplified representation of the interactions for cold atoms is useful because the large de Broglie wavelengths of the atoms makes them insensitive to the range of interatomic interactions. As a consequence, the low-energy behavior of the atoms can be described to a good approximation by zero-range interactions.

A scattering model with local interactions can be described by a *local quantum field theory*. A formulation in terms of a quantum field theory is useful because the same framework describes the 2-body, higher few-body, and many-body problems. Quantum field theories with local interaction terms are particularly convenient, because theoretical methods for dealing with such theories are well developed. Much of the stimulus for this development has come from the success of local relativistic quantum field theories in describing elementary particles. One of the complications of local quantum field theories is that they are inherently singular at short distances, but this problem can be handled using the machinery of *renormalization*.

In this review, we present a unified treatment of scattering models that can be used to describe the low-energy behavior of atoms or other nonrelativistic particles with short-range interactions. We restrict our attention for the most part to bosons with the same mass and with S-wave interactions only. The extensions to fermions, to particles with different masses, and to interactions in higher angular momentum channels are straightforward using the formalism

of quantum field theory. In the simplest scattering models, the only degrees of freedom are atoms that are all in the same spin state. We also consider scattering models whose degrees of freedom include atoms in other spin states or diatomic molecules.

We define the physical parameters of each scattering model by specifying the S-wave phase shift for the spin state of primary interest. We formulate the model as a local quantum field theory with an ultraviolet cutoff. The renormalizations that relate the coupling constants of the quantum field theory to the physical parameters of the scattering model are determined. The Green's function that describes the evolution of a 2-atom system is derived analytically. It is used to determine the T-matrix elements for atom-atom scattering and the binding energies of diatomic molecules.

We begin the review in Sec. 2 by describing a *fundamental theory* that provides an extremely accurate description of the low-energy behavior of alkali atoms. We then give a general discussion of scattering models in Sec. 3. In Sec. 4, we discuss the Zero-Range Model, whose only interaction parameter in the 2-atom sector is the scattering length. In Sec. 5, we discuss the *Effective Range Model*, which has a second interaction parameter. Other scattering models whose only degrees of freedom are an atom in a single spin state are described briefly in Sec. 6. In Sec. 7, we discuss the *Two-Channel Model*, which describes atoms that can be in either of two spin states. In Sec. 8, we describe the *Resonance Model*, in which a diatomic molecule enters as an additional degree of freedom.

2 The Fundamental Theory

In this section, we describe the *fundamental theory* that provides an extremely accurate description of atoms with energies small compared to the splitting between the ground state of the atom and its first electronic excitation. To be specific, we focus on alkali atoms. These atoms have been used extensively in cold atom experiments, because they have properties that make it particularly easy to cool them to ultralow temperatures using current technology, such as laser cooling and evaporative cooling.

2.1 Hamiltonian

The alkali atoms H, Li, Na, K, Rb, Cs, and Fr can be labeled by an integer $n = 1, 2, 3, 4, 5, 6$, and 7. The electronic structure of the n^{th} alkali atom can be roughly approximated by a single valence electron in the nS state of a Coulomb field created by the closed shells of the inner electrons and the

nucleus, which together have total electric charge +1. Thus the energy scale of the first electronic excitation of the Rb atom can be estimated from the hydrogen spectrum: $E_{\text{electronic}} \approx E_{\text{Rydberg}}/n^2$, where $E_{\text{Rydberg}} = 13.6$ eV.

An alkali atom in its electronic ground state has multiple spin states. There are two contributions to its spin: the electronic spin \mathbf{S} with quantum number $s = \frac{1}{2}$ and the nuclear spin \mathbf{I} with quantum number i . The $2(2i + 1)$ spin states can be labeled $|m_s, m_i\rangle$, where m_s and m_i specify the eigenvalues of S_z and I_z . The Hamiltonian for a single atom includes a *hyperfine term* that can be expressed in the form

$$H_{\text{hyperfine}} = \frac{2E_{\text{hf}}}{(2i + 1)\hbar^2} \mathbf{I} \cdot \mathbf{S}. \quad (1)$$

This term splits the ground state of the atom into two hyperfine multiplets with energies differing by E_{hf} . The eigenstates can be labeled by the eigenvalues of the hyperfine spin $\mathbf{F} = \mathbf{I} + \mathbf{S}$. The associated quantum numbers f and m_f specify the eigenvalues of \mathbf{F}^2 and F_z . The eigenvalues of $H_{\text{hyperfine}}$ are

$$E_{f, m_f} = \frac{f(f + 1) - i(i + 1) - \frac{3}{4}}{2i + 1} E_{\text{hf}}. \quad (2)$$

The hyperfine multiplet consists of $2i + 2$ states with $f = i + \frac{1}{2}$ and $2i$ states with $f = i - \frac{1}{2}$.

In the presence of a magnetic field $\mathbf{B} = B\hat{\mathbf{z}}$, the Hamiltonian for a single atom has a *magnetic term*. The magnetic moment $\boldsymbol{\mu}$ of the atom is dominated by the term proportional to the spin of the electron: $\boldsymbol{\mu} = \mu \mathbf{S}/(\frac{1}{2}\hbar)$. The magnetic term in the Hamiltonian can be expressed in the form

$$H_{\text{magnetic}} = -\frac{2\mu}{\hbar} \mathbf{S} \cdot \mathbf{B}. \quad (3)$$

If $B \neq 0$, this term splits the two hyperfine multiplets into $2(2i + 1)$ hyperfine states. In a weak magnetic field satisfying $\mu B \ll E_{\text{hf}}$, each hyperfine multiplet is split into $2f + 1$ equally-spaced Zeeman levels $|f, m_f\rangle$. In a strong magnetic field satisfying $\mu B \gg E_{\text{hf}}$, the states are split into a set of $2i + 1$ states with $m_s = -\frac{1}{2}$ whose energies increase linearly with B and a set of $2i + 1$ states with $m_s = +\frac{1}{2}$ whose energies decrease linearly with B . Each of those states is the continuation in B of a specific hyperfine state $|f, m_f\rangle$ at small B . It is convenient to label the states by the hyperfine quantum number f and m_f for general B , in spite of the fact that those states are not eigenstates of \mathbf{F}^2 if $B \neq 0$. We denote the eigenstates of $H_{\text{hyperfine}} + H_{\text{magnetic}}$ by $|f, m_f; B\rangle$ and their eigenvalues by $E_{f, m_f}(B)$. The two eigenstates with the maximal value of $|m_f|$ are independent of B :

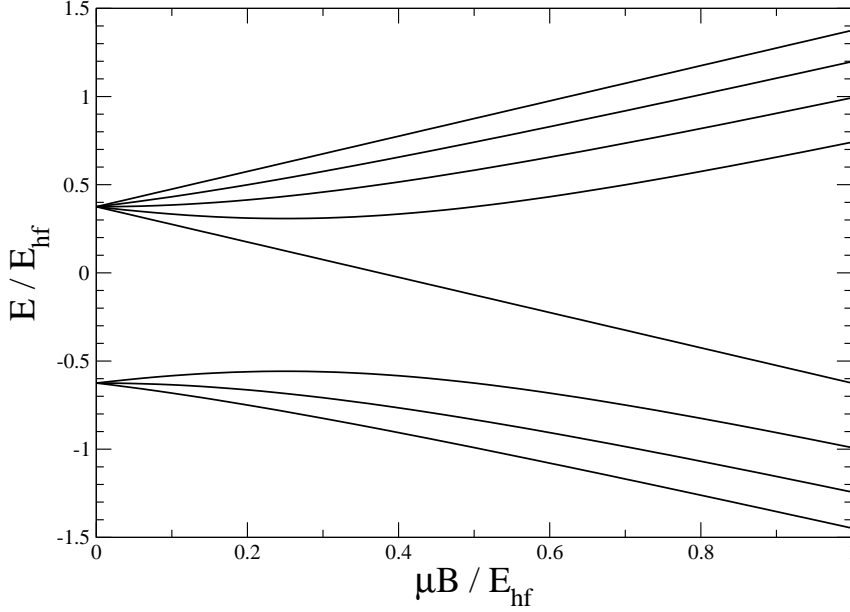


Fig. 1. The hyperfine energy levels as a function of the magnetic field for an alkali atom with $i = \frac{3}{2}$, such as ^{87}Rb .

$$\left| f = i + \frac{1}{2}, m_f = \pm(i + \frac{1}{2}); B \right\rangle = \left| m_s = \pm\frac{1}{2}, m_i = \pm i \right\rangle. \quad (4)$$

Their eigenvalues are exactly linear in B :

$$E_{f,m_f}(B) = \frac{i}{2i+1} E_{\text{hf}} \mp \mu B. \quad (5)$$

If $B \neq 0$, each of the other eigenstates $|f, m_f; B\rangle$ is a linear superposition of the two states $|f = i - \frac{1}{2}, m_f\rangle$ and $|f = i + \frac{1}{2}, m_f\rangle$.

As an illustration, we take ^{87}Rb atoms, whose nuclear spin quantum number is $i = \frac{3}{2}$. Since Rb is the 5th alkali atom, the energy scale of its first electronic excitation is approximately $E_{\text{Rydberg}}/5^2 \approx 0.55$ eV. At $B = 0$, the electronic ground state is split into hyperfine multiplets with $f = 1$ and $f = 2$, with the $f = 2$ multiplet higher in energy by $E_{\text{hf}} = 2.83 \times 10^{-5}$ eV. Thus the hyperfine splitting is more than 4 orders of magnitude smaller than the energy scale for electronic excitations. The magnetic moment μ of a Rb atom is approximately that of an electron: $\mu \approx 2\mu_B$, where μ_B is the Bohr magneton. The magnetic energy scale μB is comparable to E_{hf} when B is about 2400 Gauss. The dependence of the hyperfine energy levels on the magnetic field is illustrated in Fig. 1.

If the atoms have sufficiently low energy that none of their electronic excita-

tions can be excited, they can be described as point particles with multiple spin states that interact nonlocally through a potential. In the case of two alkali atoms, their interactions at sufficiently low energies can be described by the *Born-Oppenheimer potentials* $V_s(r)$ and $V_t(r)$ for atoms whose valence electrons are in *spin-singlet* and *spin-triplet* states, respectively. The spin-dependent potential can be written as an outer-product operator acting on the space of 2-atom spin states $|m_s, m_i\rangle \otimes |m'_s, m'_i\rangle$:

$$\begin{aligned} \mathcal{V}(r) = & V_t(r) \left[\frac{3}{4} (1 \otimes 1) + (\sum_i S^i \otimes S^i) / \hbar^2 \right] \\ & + V_s(r) \left[\frac{1}{4} (1 \otimes 1) - (\sum_i S^i \otimes S^i) / \hbar^2 \right]. \end{aligned} \quad (6)$$

The asymptotic behaviors of the two potentials at large r are

$$V_t(r), V_s(r) \longrightarrow E_0 - \frac{C_6}{r^6}, \quad (7)$$

where E_0 is the scattering threshold for two atoms in the absence of the hyperfine and magnetic interactions. The scattering thresholds are split by the hyperfine and magnetic interactions in Eqs. (1) and (3). The threshold for two atoms in the states $|f, m_f; B\rangle$ and $|f', m'_f; B\rangle$ is $2E_0 + E_{f, m_f}(B) + E_{f', m'_f}(B)$.

There are also 3-body and higher n -body interactions between atoms. Their effects are generally believed to be negligible in most cases, and we will ignore them. We will also ignore relativistic effects and retardation effects, which change the ultimate asymptotic behavior of the van der Waals potential from $1/r^6$ to $1/r^7$.

The nucleus of an atom with atomic number Z and atomic mass number A contains Z protons and $A - Z$ neutrons. The atom also contains Z electrons to neutralize the electric charge. Thus the total number of fermionic constituents in the atom is $A + Z$. The atom is a boson if $A + Z$ is even and a fermion if $A + Z$ is odd. In the case of alkali atoms, the atomic number Z is always odd. Thus an alkali atom is a boson if A is odd and a fermion if A is even.

If two atoms are in the same spin state $|f, m_f; B\rangle$, their wavefunction $\psi(\mathbf{r}_1, \mathbf{r}_2)$ must satisfy a *symmetrization* condition. If the atom is a boson, the wavefunction must be symmetric under interchange of the two coordinates: $\psi(\mathbf{r}_2, \mathbf{r}_1) = +\psi(\mathbf{r}_1, \mathbf{r}_2)$. If the atom is a fermion, the wavefunction must be antisymmetric under interchange of the two coordinates. More generally, two atoms can be in superpositions of the various hyperfine states, in which case their wavefunction has multiple components $\psi_{m_{s1}m_{i1}, m_{s2}m_{i2}}(\mathbf{r}_1, \mathbf{r}_2)$. The symmetrization condition must be applied to the spin quantum numbers as well as to the coordinate dependence of the wavefunction. If the atom is a boson, the components of the wavefunction must satisfy

$$\psi_{m_{s2}m_{i2},m_{s1}m_{i1}}(\mathbf{r}_2, \mathbf{r}_1) = +\psi_{m_{s1}m_{i1},m_{s2}m_{i2}}(\mathbf{r}_1, \mathbf{r}_2). \quad (8)$$

We can now specify the fundamental theory. The Hamiltonian is the sum of a one-body term for every particle and a 2-body term for every pair of particles. The one-body term is the sum of the kinetic energy $\mathbf{P}^2/(2m)$, the hyperfine term in Eq. (1), and the magnetic term in Eq. (3). The 2-body potentials are given in Eq. (6). The bosonic or fermionic nature of the atoms is implemented through constraints on the states. If the atom is a boson, the N -particle wavefunction must be symmetric under interchange of any pair of atoms. If the atom is a fermion, the N -particle wavefunction must be antisymmetric under such an interchange.

2.2 Quantum field theory formulation

The fundamental theory can be formulated as a *quantum field theory*. This formulation involves $2(2i+1)$ quantum fields $\psi_{m_s m_i}(\mathbf{r})$ that can be arranged into a column vector $\Psi(\mathbf{r})$. The Hamiltonian is

$$H_{\text{fun}} = \int d^3r \left(\frac{1}{2m} \nabla \Psi^\dagger \cdot \nabla \Psi + \frac{2E_{\text{hf}}}{2i+1} \Psi^\dagger \mathbf{I} \cdot \mathbf{S} \Psi - 2\mu \mathbf{B} \cdot \Psi^\dagger \mathbf{S} \Psi \right) + \frac{1}{2} \int d^3r_1 \int d^3r_2 (\Psi(\mathbf{r}_1) \otimes \Psi(\mathbf{r}_2))^\dagger \mathcal{V}(r_{12}) (\Psi(\mathbf{r}_1) \otimes \Psi(\mathbf{r}_2)), \quad (9)$$

where $r_{12} = |\mathbf{r}_1 - \mathbf{r}_2|$. We have set $\hbar = 1$ to simplify the expression. Dimensional analysis can be used to reintroduce \hbar if desired. The quantum fields $\psi_{m_s m_i}(\mathbf{r})$ satisfy equal-time commutation relations. If the atom is a boson, the commutation relations are

$$[\psi_{m_s m_i}(\mathbf{r}), \psi_{m'_s m'_i}(\mathbf{r}')] = 0, \quad (10a)$$

$$[\psi_{m_s m_i}(\mathbf{r}), \psi_{m'_s m'_i}^\dagger(\mathbf{r}')] = \delta_{m_s m'_s} \delta_{m_i m'_i} \delta^3(\mathbf{r} - \mathbf{r}'). \quad (10b)$$

If the atom is a fermion, the commutation relations are replaced by anti-commutation relations. The commutation relations imply that the quantum field $\psi_{m_s m_i}(\mathbf{r})$ annihilates an atom in the spin state $|m_i, m_s\rangle$ at the point \mathbf{r} . They also enforce the constraint that quantum states must be symmetric under interchange of two atoms in the same spin state.

The fundamental theory has several symmetries:

- *phase symmetry*. The Hamiltonian H_{fun} is invariant under phase transformations: $\Psi(\mathbf{r}) \rightarrow e^{i\theta} \Psi(\mathbf{r})$. This symmetry is associated with the conservation of the number of atoms.

- *translational symmetry*. If the magnetic field $\mathbf{B}(t)$ is homogeneous, H_{fun} is invariant under translations in space: $\mathbf{r} \rightarrow \mathbf{r} + \mathbf{a}$. This implies the conservation of the total momentum \mathbf{P} .
- *time translational symmetry*. If the magnetic field $\mathbf{B}(\mathbf{r})$ is static, the theory is invariant under translations in time: $t \rightarrow t + a$. This implies the conservation of the total energy E , which is the eigenvalue of the Hamiltonian H_{fun} .
- *rotational symmetry*. The Hamiltonian is invariant under rotations generated by the total angular momentum operator $\mathbf{J} = \mathbf{L} + \mathbf{S} + \mathbf{I}$, where \mathbf{L} is the orbital angular momentum, provided the magnetic field \mathbf{B} is also transformed by the rotation. If $\mathbf{B} = 0$, this symmetry implies the conservation of the total angular momentum \mathbf{J} . If $\mathbf{B} = B\hat{\mathbf{z}}$, it implies the conservation of the component J_z .
- *parity symmetry*. The Hamiltonian is invariant under the reflection $\mathbf{r} \rightarrow -\mathbf{r}$.

The fundamental theory also has *Galilean symmetry*. Since the Hamiltonian is the generator of translations in time, the column vector of quantum fields can be extended to a time-dependent operator $\Psi(\mathbf{r}, t)$:

$$\Psi(\mathbf{r}, t) = e^{iH_{\text{fun}}t}\Psi(\mathbf{r})e^{-iH_{\text{fun}}t}. \quad (11)$$

The transformation of this time-dependent operator under a Galilean boost with velocity vector \mathbf{v} is

$$\Psi(\mathbf{r}, t) \longrightarrow e^{im\mathbf{v}\cdot\mathbf{r}-i(\frac{1}{2}mv^2)t}\Psi(\mathbf{r} - \mathbf{v}t, t). \quad (12)$$

This symmetry is not associated with a conservation law, because its generators do not commute with the Hamiltonian.

If we restrict our attention to low energies with respect to a given scattering threshold, the fundamental theory has additional approximate symmetries. If the atoms have sufficiently low kinetic energy, their total orbital angular momentum \mathbf{L} can be neglected. If $\mathbf{B} = 0$, the total hyperfine spin $\mathbf{F} = \mathbf{I} + \mathbf{S}$ is then conserved. If there is a nonzero magnetic field $\mathbf{B} = B\hat{\mathbf{z}}$, the component F_z is conserved. The restriction on the energy may also impose a restriction on the possible spin states of the atoms. In this case, the conservation of total atom number may be replaced by a more restrictive conservation law. If $B = 0$, the energy restriction could allow only atoms in a specific hyperfine multiplet with quantum number f , in which case the total number of atoms in those $2f + 1$ hyperfine states will be conserved. If B is large, the energy restriction may require all the atoms to be in the same spin state, in which case the number of atoms in that spin state will be conserved.

2.3 Scattering

If two atoms in the hyperfine states $|f_1, m_{f1}; B\rangle$ and $|f_2, m_{f2}; B\rangle$ collide, they can either scatter elastically or they can scatter into a different pair of hyperfine states $|f'_1, m'_{f1}; B\rangle$ and $|f'_2, m'_{f2}; B\rangle$. The scattering rate for each scattering channel is determined by the T -matrix element, which is a function of the relative wavenumbers \mathbf{k} and \mathbf{k}' for the initial and final states. If the collision energy relative to the scattering threshold is sufficiently small, elastic scattering is dominated by the S -wave orbital angular momentum channel and the T -matrix element $\mathcal{T}_{f_1 m_{f1}, f_2 m_{f2}}(k)$ for elastic scattering reduces to a function of $k = |\mathbf{k}| = |\mathbf{k}'|$ only. The low-energy limit of the T -matrix element is given by the scattering lengths for the hyperfine channel. If the two hyperfine states are distinct, we denote the scattering length by $a_{f_1 m_{f1}, f_2 m_{f2}}$. The low-energy limit of the T -matrix element is

$$\mathcal{T}_{f_1 m_{f1}, f_2 m_{f2}}(k) \longrightarrow -\frac{4\pi}{m} a_{f_1 m_{f1}, f_2 m_{f2}} \quad \text{as } k \rightarrow 0. \quad (13)$$

If the two atoms are in the same hyperfine state $|f, m_f; B\rangle$, we denote the scattering length by $a_{f m_f}$. The low-energy limit of the T -matrix element is

$$\mathcal{T}_{f m_f, f m_f}(k) \longrightarrow -\frac{8\pi}{m} a_{f m_f} \quad \text{as } k \rightarrow 0. \quad (14)$$

If the atoms are fermions, the scattering length $a_{f m_f}$ vanishes because the wavefunction for an S -wave state must be symmetric under interchange of the coordinates. The cross section for the scattering of distinct hyperfine states are obtained by squaring the T -matrix element $\mathcal{T}_{f_1 m_{f1}, f_2 m_{f2}}(k)$ and multiplying it by the flux factor $m/(2k)$ and by the phase space factor $mk/(2\pi)$. If the two atoms are in the same hyperfine state, the phase space factor is multiplied by a factor of $\frac{1}{2}$ to compensate for the double-counting of the states of the identical particles. Thus the low-energy limit of the cross section for the elastic scattering of two atoms in the $|f, m_f; B\rangle$ hyperfine state is

$$\sigma_{\text{elastic}}(E) \longrightarrow 8\pi |a_{f m_f}|^2 \quad \text{as } E \rightarrow 0. \quad (15)$$

In the absence of the hyperfine and magnetic interactions, scattering through the spin-singlet and spin-triplet potentials in Eq. (6) determines the spin-singlet and spin-triplet scattering lengths a_s and a_t . The spin-triplet scattering length a_t is the scattering length for a pair of atoms that are both in the same hyperfine state given in Eq. (4). The only effect of the hyperfine and magnetic terms on this channel is to change the scattering threshold. If it were not for the hyperfine term in Eq. (1), the scattering lengths for all the other hyperfine

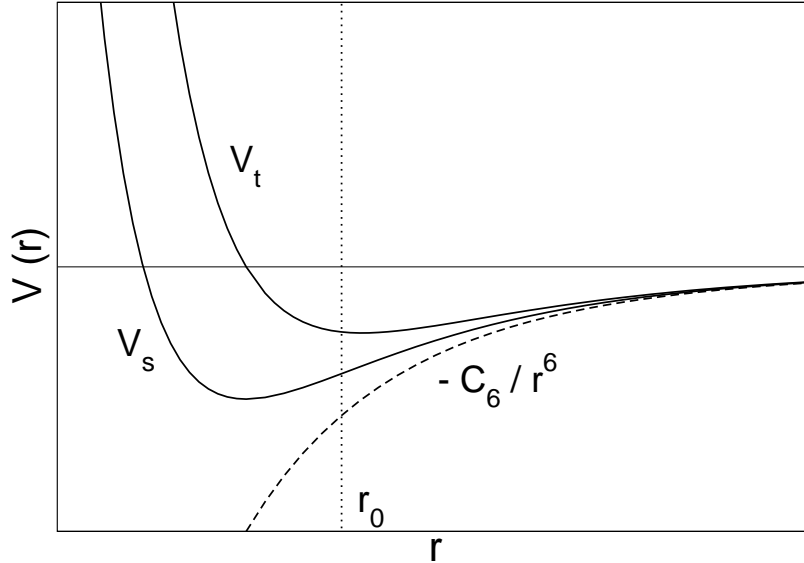


Fig. 2. Qualitative behavior of the spin-singlet potential (lower solid line) and the spin-triplet potential (upper solid line). The low-energy scattering properties can be reproduced by replacing both potentials by the van der Waals potential $-C_6/r^6$ with a boundary condition at $r = r_0$ such that the spin-singlet and spin-triplet scattering lengths have the correct values a_s and a_t .

channels could be expressed as linear combinations of a_s and a_t using Clebsch-Gordon coefficients. Because of the hyperfine term, it is necessary to solve the coupled-channel Schrödinger equation numerically to determine the scattering lengths for all the other hyperfine channels. However, if the scattering lengths a_s and a_t are known, there is a simple approximation to the coupled-channel problem that reproduces the low-energy scattering observables, including the scattering lengths, quite accurately [1]. As illustrated in Fig. 2, the spin-singlet and spin-triplet potentials $V_s(r)$ and $V_t(r)$ in Eq. (6) can be replaced by their asymptotic forms in Eq. (7) together with boundary conditions at a small separation r_0 . The boundary conditions are tuned so that the spin-singlet and spin-triplet scattering lengths have the desired values a_s and a_t for $B = 0$ and $E_{\text{hf}} = 0$. Those same boundary conditions are then used for nonzero values of B and E_{hf} . Thus the low-energy scattering problem for all the hyperfine channels is essentially determined by just 5 parameters: a_s , a_t , C_6 , E_{hf} , and μB .

We now focus on a specific hyperfine channel. To be definite, we take the alkali atom to be a boson. We also take the two atoms to be in the same hyperfine state $|f, m_f; B\rangle$, so they are identical bosons. We choose the origin of energy to

be the scattering threshold for that channel: $2E_0 + 2E_{f,m_f}(B)$. The T-matrix element for S-wave scattering of two particles with collision energy $E = k^2/m$ can be expressed in the form

$$\mathcal{T}(k) = \frac{8\pi}{m} \frac{1}{k \cot \delta_0(k) - ik}, \quad (16)$$

where $\delta_0(k)$ is the S-wave phase shift. If there are no lower hyperfine channels into which the atoms can scatter, the unitarity of the S-matrix implies that the phase shift is real valued. The low-energy behavior of the phase shift is given by the *effective range expansion*:

$$k \cot \delta_0(k) = -1/a + \frac{1}{2}r_s k^2 + \dots, \quad (17)$$

which defines the *scattering length* $a = a_{f,m_f}$ and the *effective range* r_s . Taking the limit $k \rightarrow 0$ in Eq. (16) and using Eq. (17), we recover the limiting expression for the T-matrix element in Eq. (14).

If the fundamental theory had only short-range potentials, $k \cot \delta_0(k)$ would be an analytic function of k^2 at $k = 0$ and it would therefore have a power series expansion in k^2 . However, the asymptotic behavior of the potentials $V_s(r)$ and $V_t(r)$, as given in Eq. (7), is $1/r^6$. As a consequence, beginning at order k^4 , there are logarithms of k in the coefficients of the powers of k . Thus $k \cot \delta_0(k)$ has a well-behaved expansion in powers of k^2 only to order k^2 . Thus the scattering length and the effective range defined by Eq. (17) are the only well-defined coefficients in the effective range expansion for atoms.

The important energy scales for low-energy alkali atoms include the hyperfine splitting $E_{\text{hyperfine}}$, the magnetic energy scale μB , and the van der Waals energy scale defined by

$$E_{\text{vdw}} = (m^3 C_6 / \hbar^6)^{-1/2}. \quad (18)$$

For Rb atoms, the van der Waals energy scale is $E_{\text{vdW}} = 6.4 \times 10^{-9}$ eV. This is more than 3 orders of magnitude smaller than the hyperfine splitting E_{hf} . The magnetic energy scale μB is comparable to E_{vdW} when the magnetic field is about 0.54 Gauss. The van der Waals energy scale corresponds to a temperature of 7.4×10^{-5} K. We consider atoms to be *ultracold* if their kinetic energies are much smaller than the van der Waals energy scale. In subsequent sections, we will review scattering models that can describe such ultracold atoms.

2.4 Large scattering length

The natural scale for the scattering length a of a specific hyperfine state is the van der Waals length defined by

$$\ell_{\text{vdw}} = (mC_6/\hbar^2)^{1/4}. \quad (19)$$

A scattering length can be orders of magnitude larger than ℓ_{vdw} only if there is a fine-tuning of some parameter in the Hamiltonian. If $|a|$ is much larger than ℓ_{vdw} , we refer to a as a *large scattering length*. If a is large, ultracold atoms have an important energy scale that is much smaller than the van der Waals energy scale E_{vdw} , namely $\hbar^2/(ma^2)$.

For particles with short-range interactions, the scattering length a is considered to be large if its absolute value is much larger than the range. Particles with large scattering lengths have universal low-energy properties that depend on the scattering length but are insensitive to other details of the interactions. The known universal properties have been summarized in a recent review [2]. In the case of atoms, the relevant range is the van der Waals length scale ℓ_{vdw} defined in Eq. (19). In the 2-atom sector, the universal properties are rather simple. The cross section for elastic scattering of bosonic atoms in the same spin state with energy in the region $|E| \ll E_{\text{vdw}}$, where E_{vdw} is the van der Waals energy scale defined in Eq. (18), is given by the universal formula

$$\sigma_{\text{elastic}}(E) = \frac{8\pi a^2}{1 + ma^2 E}. \quad (20)$$

Shallow bound states whose binding energies are much smaller than E_{vdw} are also universal. If $a < 0$, there are no such bound states. If $a > 0$, there is a single shallow bound state with binding energy

$$E_D = 1/(ma^2). \quad (21)$$

We will refer to this state as the *shallow dimer*.

The natural scale for the scattering lengths a_s and a_t is the van der Waals length defined in Eq. (19). The scattering length a_s or a_t can be much larger than ℓ_{vdw} only if the depth of the potential $V_s(r)$ or $V_t(r)$ is tuned so that there is a bound state very close to the threshold. If a_s or a_t is large, several of the scattering lengths a_{fm_f} of the hyperfine channels will also be large. Examples of alkali atoms that have large scattering lengths at zero magnetic field are ^6Li ($a_t \approx -2160 a_0$), ^{85}Rb ($a_s \approx +2800 a_0$), and ^{133}Cs ($a_t \approx +2400 a_0$).

A large scattering length a_{fm_f} in a specific hyperfine channel can be obtained by tuning the magnetic field B to a *Feshbach resonance* B_i . If the magnetic field is near B_i , there is a diatomic molecule near the scattering threshold for two atoms in the $|f, m_f; B\rangle$ hyperfine state. The diatomic molecule is a bound state of atoms in a spin state with a higher threshold. Since the magnetic moment of the diatomic molecule differs from twice the magnetic moment of the $|f, m_f; B\rangle$ atom, the energy of the molecule can be made to cross the scattering threshold by changing the magnetic field B . The *Feshbach resonance* occurs at the value B_i for which the molecule is at resonance with two atoms at the scattering threshold. The existence of Feshbach resonances in Cs atoms was first pointed out by Tiesinga, Verhaar, and Stoof [3]. The first Feshbach resonances to be observed were the resonances at 853 G and 907 G for ^{23}Na atoms in the $|1, -1\rangle$ hyperfine level [4] and the resonance at 155 G for ^{85}Rb atoms in the $|2, -2\rangle$ hyperfine level [5]. The physics of Feshbach resonances in cold atoms has been summarized in a recent review [6].

At a generic value B_0 of the magnetic field, the scattering length $a(B)$ for a specific hyperfine channel varies slowly as a function of the magnetic field B . It can therefore be expanded as a power series around $B = B_0$:

$$a(B) = a(B_0) + a'(B_0)(B - B_0) + \dots \quad (22)$$

At a Feshbach resonance, the scattering length is not a smooth function of B . When the magnetic field is well below the Feshbach resonance B_i , the scattering length has some off-resonant value a_{bg} . As B increases through the value B_i , $a(B)$ diverges to $+\infty$ or $-\infty$, jumps discontinuously to $-\infty$ or $+\infty$, and then approaches the original off-resonant value a_{bg} . The scattering length must pass through zero at some value of B , either before or after B_i . If we denote that value by $B_i + \Delta_i$, the scattering length can be expressed as

$$a(B) = a_{\text{bg}}(B) \left(1 - \frac{\Delta_i}{B - B_i} \right), \quad (23)$$

where $a_{\text{bg}}(B)$ is a smooth function of the magnetic field that can be expanded as a power series around B_i as in Eq. (22). The parameters B_i and Δ_i are convenient, because it is often possible to measure the locations of divergences and zeroes of the scattering length more accurately than its value $a(B)$ at any particular value of B .

3 Scattering models

The fundamental theory described in Sec. 2 provides an extremely accurate description of systems consisting of atoms in any of the hyperfine states as long as their energies are small compared to the electronic excitation energy of the atom. If we restrict our attention to ultracold atoms, whose energies relative to a specific scattering threshold are small compared to the van der Waals energy scale E_{vdW} defined in Eq. (18), we can describe the system accurately using a much simpler model. The effects of virtual atoms whose energies are far from the scattering threshold can be taken into account through the parameters of the model.

We take the atoms of primary interest to be those in a specific hyperfine state $|f, m_f; B\rangle$. We choose the zero of energy to be the scattering threshold for atoms in that hyperfine state. We restrict our attention to ultracold atoms whose energies satisfy $|E| \ll E_{\text{vdW}}$. If $\mu B \ll E_{\text{vdW}}$, this energy constraint can be satisfied by atoms in any of the $2f + 1$ spin states in the same hyperfine multiplet. For larger values of B , only atoms in the single hyperfine state $|f, m_f; B\rangle$ satisfy this energy constraint.

3.1 Potential models

One class of models that can be used to describe the behavior of ultracold atoms in the spin state of interest is *potential models*. A potential model is specified by interaction potentials between the constituents of the model. In the simplest potential models, the only constituents are atoms in the spin state of interest. In this case, the potential model is specified by a single potential $V(r)$. The potential $V(r)$ must be tuned so that the solutions to the single-channel Schrödinger equation for that potential give the same results for low-energy scattering cross sections and low-energy bound states as the solution to the coupled-channel Schrödinger equation for the fundamental theory. The potential $V(r)$ need not resemble either of the potentials $V_s(r)$ or $V_t(r)$ in the fundamental theory as long as it accurately reproduces low-energy observables for atoms in the spin state of interest. If we restrict our attention to sufficiently low energies that the scattering length a is the only relevant interaction parameter, then all that is required is that the potential be short-ranged and give the correct scattering length.

A potential model can be formulated as a quantum field theory. If the only constituents in the model are atoms in a single hyperfine state $|f, m_f; B\rangle$, there is a single quantum field $\psi(\mathbf{r})$ which annihilates atoms in that hyperfine state. The Hamiltonian is

$$\begin{aligned}
H_{\text{pot}} = & \int d^3r \frac{1}{2m} \nabla \psi^\dagger \cdot \nabla \psi \\
& + \frac{1}{2} \int d^3r_1 \int d^3r_2 \psi(\mathbf{r}_1)^\dagger \psi(\mathbf{r}_2)^\dagger V(r_{12}) \psi(\mathbf{r}_1) \psi(\mathbf{r}_2).
\end{aligned} \tag{24}$$

The time-dependent quantum field $\psi(\mathbf{r}, t)$ satisfies equal-time commutation relations. If the atom is a boson, the commutation relations are

$$[\psi(\mathbf{r}, t), \psi(\mathbf{r}', t)] = 0, \tag{25a}$$

$$[\psi(\mathbf{r}, t), \psi^\dagger(\mathbf{r}', t)] = \delta^3(\mathbf{r} - \mathbf{r}'). \tag{25b}$$

A more elaborate potential model could describe $N - 1$ additional spin states of the atoms. The model would be specified by the diagonal potentials for each pair of spin states and by coupling potentials between pairs of spin states. These potentials need not resemble those of the fundamental theory as long as the solutions to the Schrödinger equation for all the coupled channels reproduce the predictions of the fundamental theory for low-energy observables involving the spin state of interest.

3.2 Scattering Models

Another class of models that can be used to describe the low-energy behavior of the atoms is *scattering models*. A scattering model can be specified by the T -matrix elements for scattering of the constituents of the model along with any additional parameters that are required to make the model well-defined. In the simplest scattering models, the only constituents are atoms in a single spin state. At sufficiently low energies, the atoms have only S-wave scattering and the T -matrix element reduces to a function $\mathcal{T}(k)$ of the magnitude of the relative momentum k only. Since it is specified in terms of the low-energy observables $\mathcal{T}(k)$, a scattering model provides a particularly natural description for ultracold atoms.

A more elaborate scattering model could include other spin states of the atom as additional degrees of freedom. In this case, the T -matrix elements for all the pairs of spin states could be part of the specification of the model. In contrast to potential models, diatomic molecules can also be included as explicit degrees of freedom in a scattering model. In this case, T -matrix elements involving the diatomic molecules could also be part of the specification of the model.

3.3 Hamiltonian quantum field theories

A scattering model can be formulated as a quantum field theory. If the T-matrix element $\mathcal{T}(k)$ that is part of the specification of the scattering model is an analytic function of k^2 at $k = 0$, the T-matrix element can be reproduced by a *local quantum field theory*. A local quantum field theory is one whose interactions only involve the quantum fields and their derivatives at the same point in space. If a local quantum field theory has a Hamiltonian formulation, its Hamiltonian can be expressed as the integral over space of a Hamiltonian density:

$$H = \int d^3r (\mathcal{H}_{\text{free}} + \mathcal{H}_{\text{int}}). \quad (26)$$

If the quantum field $\psi(\mathbf{r})$ that annihilates atoms in the spin state of interest is the only quantum field in the model, the free term in the Hamiltonian density is

$$\mathcal{H}_{\text{free}} = \frac{1}{2m} \nabla \psi^\dagger \cdot \nabla \psi. \quad (27)$$

The interaction term in the Hamiltonian density must be a polynomial in ψ and ψ^\dagger and their gradients, such as

$$\begin{aligned} \mathcal{H}_{\text{int}} = & \frac{1}{4} \lambda_0 (\psi^\dagger)^2 \psi^2 \\ & + \frac{1}{4} \rho_0 \left((\psi^\dagger)^2 \nabla \psi \cdot \nabla \psi + 2 \psi^\dagger \psi \nabla \psi^\dagger \cdot \nabla \psi + \psi^2 \nabla \psi^\dagger \cdot \nabla \psi^\dagger \right) + \dots \end{aligned} \quad (28)$$

One advantage of a Hamiltonian quantum field theory is that it guarantees that the space of quantum states is a Hilbert space. Since the Hamiltonian H is a hermitian operator, its eigenstates $|n\rangle$ form a complete set of states. The completeness relation can be expressed formally as $\sum_n |n\rangle \langle n| = 1$. If we express the S-matrix in the form $\mathcal{S} = 1 + i\mathcal{T}$, the completeness relation can be used to express the unitarity condition $\mathcal{S}^\dagger \mathcal{S} = 1$ in the form

$$2 \operatorname{Im} \langle i | \mathcal{T} | i \rangle = \sum_n |\langle n | \mathcal{T} | i \rangle|^2. \quad (29)$$

This form of the unitarity condition is called the *Optical Theorem*. Note that the right side is the sum of positive-definite terms.

3.4 Lagrangian quantum field theories

It is sometimes useful to consider a more general class of quantum field theories that have a Lagrangian formulation but do not necessarily have a Hamiltonian formulation. The Lagrangian for a local quantum field theory can be expressed as the integral over space of a Lagrangian density:

$$L = \int d^3r (\mathcal{L}_{\text{free}} + \mathcal{L}_{\text{int}}). \quad (30)$$

If the quantum field $\psi(\mathbf{r})$ that annihilates atoms in the spin state of interest is the only quantum field in the model, the free term in the Lagrangian density is

$$\mathcal{L}_{\text{free}} = \frac{1}{2}i \left(\psi^\dagger \frac{\partial}{\partial t} \psi - \frac{\partial}{\partial t} \psi^\dagger \psi \right) - \frac{1}{2m} \nabla \psi^\dagger \cdot \nabla \psi. \quad (31)$$

This form is manifestly real. If we ignore terms that are total time derivatives or total divergences, it can be written in a more compact form:

$$\mathcal{L}_{\text{free}} = \psi^\dagger \left(i \frac{\partial}{\partial t} + \frac{\nabla^2}{2m} \right) \psi. \quad (32)$$

If the quantum field theory has a Hamiltonian formulation, the interaction term in the Lagrangian density is simply $\mathcal{L}_{\text{int}} = -\mathcal{H}_{\text{int}}$. However, Lagrangian quantum field theories are a more general class of models than Hamiltonian quantum field theories. They can, for example, have interaction terms that involve time derivatives, such as

$$\mathcal{L}_{\text{int}} = \frac{1}{4}m\lambda'_0(\psi^2)^\dagger \left(i \frac{\partial}{\partial t} + \frac{\nabla^2}{4m} \right) \psi^2 + \dots \quad (33)$$

More generally, \mathcal{L}_{int} must be a polynomial in ψ , ψ^\dagger , their gradients, and their time-derivatives.

If all we have is a Lagrangian formulation of the quantum field theory, there is no guarantee that the Optical Theorem will have the form in Eq. (29), where $\text{Im} \langle i|\mathcal{T}|i \rangle$ is expressed as the sum of positive-definite terms. The general expression may have the form

$$2 \text{Im} \langle i|\mathcal{T}|i \rangle = \sum_n |\langle n|\mathcal{T}|i \rangle|^2 - \sum_m |\langle m|\mathcal{T}|i \rangle|^2, \quad (34)$$

where the states labeled $|n\rangle$ and $|m\rangle$ together form a complete set. One way to interpret such a relation is that the space of quantum states is a complex vector space with indefinite norm. The completeness relation for this vector space has the form $\sum_n |n\rangle\langle n| - \sum_m |m\rangle\langle m| = 1$. The states $|m\rangle$ can be interpreted as states with *negative norm*.

The problem of negative-norm states arises in covariant formulations of Quantum Electrodynamics. However, one can use gauge invariance to show that there is a *physical subspace* of the complex vector space spanned by the positive-norm states $|n\rangle$ such that if $|i\rangle$ is in the physical subspace, $\text{Im} \langle i|\mathcal{T}|i\rangle$ can be written as the sum of positive-definite terms:

$$2 \text{Im} \langle i|\mathcal{T}|i\rangle = \sum_{\text{physical } n} |\langle n|\mathcal{T}|i\rangle|^2. \quad (35)$$

This requires a cancelation between positive and negative terms in Eq. (34). In QED, this cancelation is guaranteed by gauge invariance. In a scattering model for atoms, there is no obvious mechanism to guarantee such a cancelation. Thus the existence of negative-definite terms in the imaginary part of a diagonal T-matrix element is more problematic.

3.5 Symmetries

The symmetries of the fundamental theory can be used to constrain the Hamiltonian or the Lagrangian of a local quantum field theory. We will give the constraints only for the simple case of a single quantum field $\psi(\mathbf{r}, t)$:

- *phase symmetry*. The phase transformation is $\psi(\mathbf{r}, t) \rightarrow e^{i\theta}\psi(\mathbf{r}, t)$. Invariance under this transformation requires that every term in \mathcal{H}_{int} or \mathcal{L}_{int} have an equal number of factors of ψ and ψ^\dagger .
- *translational symmetry*. This is implemented automatically in a local quantum field theory for which \mathcal{H}_{int} or \mathcal{L}_{int} is a function of ψ , ψ^\dagger , their gradients, and their time-derivatives.
- *time translational symmetry*. This is also implemented automatically in a local quantum field theory.
- *rotational symmetry*. If the model involves only a single quantum field $\psi(\mathbf{r}, t)$, a rotation acts only on its vector argument \mathbf{r} . The requirement of rotational symmetry is that \mathcal{H}_{int} or \mathcal{L}_{int} be a scalar under rotations. This requires each gradient ∇^i to have its index i contracted with that of another gradient ∇^i or with a Levi-Civita tensor ϵ^{ijk} .
- *parity symmetry*. This can be used to exclude terms in \mathcal{H}_{int} or \mathcal{L}_{int} with a Levi-Civita tensor.

Galilean symmetry imposes strong constraints on the interaction terms in \mathcal{H}_{int} or \mathcal{L}_{int} . The Galilean transformation with velocity vector \mathbf{v} in the fundamental theory is given in Eq. (12). The corresponding Galilean transformation for the field $\psi(\mathbf{r}, t)$ is

$$\psi(\mathbf{r}, t) \longrightarrow e^{im\mathbf{v}\cdot\mathbf{r}-i(\frac{1}{2}mv^2)t}\psi(\mathbf{r}-\mathbf{v}t, t). \quad (36)$$

One way to construct interaction terms that are Galilean invariant is to construct them out of building blocks with simple behavior under Galilean transformations. One simple building block is the product $\psi^\dagger\psi$, which is Galilean invariant. Thus terms constructed out of $\psi^\dagger\psi$ and its gradients, such as $\nabla^i(\psi^\dagger\psi)$ and $\nabla^i\nabla^j(\psi^\dagger\psi)$, are Galilean invariant. The first term in \mathcal{H}_{int} in Eq. (28) is Galilean invariant, because it can be expressed as $(\psi^\dagger\psi)^2$. The second term in \mathcal{H}_{int} is also Galilean invariant, because it can be expressed in the form $\nabla(\psi^\dagger\psi) \cdot \nabla(\psi^\dagger\psi)$.

Another simple building block is $\psi\overleftrightarrow{\nabla}^2\psi$, where the operator $\overleftrightarrow{\nabla}^2$ is defined by

$$\chi\overleftrightarrow{\nabla}^2\psi = \chi(\nabla^2\psi) - 2(\nabla\chi) \cdot (\nabla\psi) + (\nabla^2\chi)\psi. \quad (37)$$

The operator $\psi\overleftrightarrow{\nabla}^2\psi$ transforms under Galilean transformations in the same way as ψ^2 . A further set of simple building blocks is the combination $[i\frac{\partial}{\partial t} + \nabla^2/(2Nm)]\psi^N$, where $N = 1, 2, \dots$. They transform under Galilean transformations in the same way as ψ^N . This combination with $N = 1$ appears in the expression for $\mathcal{L}_{\text{free}}$ in Eq. (32). This combination with $N = 2$ appears in the interaction term in Eq. (33).

If the energy restriction allows atoms in multiple spin states related by a symmetry, the symmetry can be imposed on the corresponding quantum fields $\psi_m(\mathbf{r}, t)$. For example, if $B = 0$, the $2f + 1$ spin states in a hyperfine multiplet form an irreducible $(2f + 1)$ -dimensional representation of the $SU(2)$ symmetry group of angular momentum. There is also a $U(1)$ symmetry corresponding to multiplying all the fields $\psi_m(\mathbf{r}, t)$ by the same phase.

3.6 Two-body observables

In a quantum field theory, physical observables can be conveniently encoded in the correlation functions of the theory. The physical observables in the 2-atom sector can be encoded in the amputated connected Green's function \mathcal{A} for two atoms in the asymptotic past to evolve into two atoms in the asymptotic future. In general, this amplitude is a function of the energies E_1 and E_2 and

the momenta \mathbf{p}_1 and \mathbf{p}_2 of the two incoming atoms and the energies E'_1 and E'_2 and the momenta \mathbf{p}'_1 and \mathbf{p}'_2 of the two outgoing atoms. The atoms can be off their energy shells: E_i need not be equal to $p_i^2/(2m)$. The total energy E and the total momentum \mathbf{P} are conserved: $E_1 + E_2 = E'_1 + E'_2 = E$ and $\mathbf{p}_1 + \mathbf{p}_2 = \mathbf{p}'_1 + \mathbf{p}'_2 = \mathbf{P}$. Galilean invariance constrains the amplitude to be a function of $E - \mathbf{P}^2/(4m)$ and the relative momenta $\mathbf{k} = \frac{1}{2}(\mathbf{p}_1 - \mathbf{p}_2)$ and $\mathbf{k}' = \frac{1}{2}(\mathbf{p}'_1 - \mathbf{p}'_2)$. We can simplify the problem by working in the center-of-mass frame $\mathbf{P} = 0$. If the energy is restricted to be low enough that there is S-wave scattering only, the amplitude in the center-of-mass frame depends only on the magnitudes of \mathbf{k} and \mathbf{k}' , so it reduces to a function $\mathcal{A}(E; k, k')$ of three variables.

The amplitude $\mathcal{A}(E; k, k')$ encodes all information about low-energy 2-atom scattering. The T-matrix element $\mathcal{T}(k)$ for the S-wave scattering of two atoms with relative momentum \mathbf{k} into two atoms with relative momentum \mathbf{k}' is obtained by evaluating $\mathcal{A}(E; k, k')$ at the on-shell point obtained by setting all the atoms on their energy shells: $E = 2(k^2/2m) = 2(k'^2/2m)$, which requires $k = k'$. The T-matrix element is

$$\mathcal{T}(k) = \mathcal{A}(k^2/m; k, k). \quad (38)$$

The cross section for the elastic scattering of two identical bosonic atoms with total kinetic energy $E = k^2/m$ is obtained by squaring the T-matrix element and multiplying by the phase space factor $mk/(4\pi)$ and by the flux factor $m/(2k)$:

$$\sigma(E) = \frac{m^2}{8\pi} |\mathcal{T}(k)|^2. \quad (39)$$

Information about S-wave bound states is also encoded in $\mathcal{A}(E; k, k')$ through its poles in the energy E . The amplitude $\mathcal{A}(E; k, k')$ is a double-valued function of the energy variable E , which takes its values on the two-sheeted complex plane with a branch point at $E = 0$ and a branch cut along the positive E axis. The interpretation of the pole in E depends on where the pole resides in the complex E plane. For simplicity, we assume that the atom has no spin states with lower energy. A pole on the negative real axis of the physical sheet of the complex energy E corresponds to a *stable bound state*. A pole on the negative real axis of the unphysical sheet is called a *virtual state*. A pole on the unphysical sheet just below the positive real axis corresponds to a *scattering resonance*.

3.7 Renormalization

One complication of local quantum field theories is that they are inherently singular at short distances. The theory is well-defined only if it is modified in some way to suppress the effects of particles that approach arbitrarily close to each other or that have arbitrarily high energy. A convenient way to do this is to impose an upper limit on the wavevector of virtual particles: $|\mathbf{k}| < \Lambda$. The variable Λ is called the *ultraviolet cutoff*. The singularities then appear in the limit $\Lambda \rightarrow \infty$. However, it is possible to avoid the singularities by using a procedure called *renormalization*. The parameters of the model, such as λ_0 and ρ_0 in Eq. (28), are made functions of Λ in such a way that the model has a well-behaved and nontrivial limit as $\Lambda \rightarrow \infty$.

There are two rather different approaches to renormalization. The simplest approach conceptually is called *Gell-Mann-Low renormalization*. This is the approach that was followed in the original development of renormalized perturbation theory for Quantum Electrodynamics. A quantum field theory model can be specified by a Hamiltonian density with a finite number of interaction terms:

$$\mathcal{H} = \mathcal{H}_{\text{free}} + \sum_{n=1}^N c_n(\Lambda) \mathcal{O}_n. \quad (40)$$

If the coupling constants $c_n(\Lambda)$ can be tuned as functions of the ultraviolet cutoff so that physical observables have well-behaved and nontrivial limits as $\Lambda \rightarrow \infty$, the model is called *renormalizable*. It may be necessary to add operators to the set $\{\mathcal{O}_1, \dots, \mathcal{O}_N\}$ or remove some of the operators to make the model renormalizable. In nonrelativistic quantum field theories in which the total number of particles cannot change, the physical observables can be classified according to the particle number. If the coupling constants can be tuned so that all N -particle observables have well-behaved limits as $\Lambda \rightarrow \infty$, the model is called *renormalizable in the N -atom sector*. If the model is renormalizable in the N -atom sector, it is renormalizable in the n -atom sector for all $n < N$. In this paper, we will for the most part consider only the constraints from renormalizability in the 2-atom sector.

The other approach to renormalization is called *Wilsonian renormalization*. This approach was followed by Ken Wilson when he developed the renormalization group to understand strongly-interacting quantum field theories. One begins by considering the most general model consistent with the symmetries. The Hamiltonian density in Eq. (40) is generalized to one with infinitely many operators \mathcal{O}_n , each with its own coupling constant $c_n(\Lambda)$. The free term $\mathcal{H}_{\text{free}}$ is included as just another operator with a coupling constant $c_{\text{free}}(\Lambda)$. We define the engineering dimension d_n of an operator \mathcal{O}_n by specifying the

dimensions of ψ and ∇ to be $\frac{3}{2}$ and 1, respectively. For this purpose, the mass m is treated as a dimensionless conversion factor. The engineering dimension of the free term in Eq. (27) is then 5. An N -atom operator with N factors of ψ , N factors of ψ^\dagger , and D factors of the gradient ∇ has engineering dimension $3N + D$. It is convenient to introduce dimensionless coupling constants $\hat{c}_n(\Lambda)$ defined by

$$\hat{c}_n(\Lambda) = \Lambda^{d_n-5} c_n(\Lambda). \quad (41)$$

The condition that low-energy observables defined by the Hamiltonian be independent of Λ defines a flow on the infinite-dimensional space of dimensionless coupling constants \hat{c}_n . This flow can have a *fixed point* whose coordinates c_n^* are independent of Λ . The corresponding fixed-point Hamiltonian \mathcal{H}^* describes a scale-invariant system. Near the fixed point, a convenient basis of operators consists of *scaling operators* \mathcal{O}_n^* that have the property that when their coupling constants are infinitesimally small, they scale as definite powers of Λ :

$$\hat{c}_n(\Lambda) \sim \Lambda^{\gamma_n}. \quad (42)$$

We refer to the exponent γ_n as the *scaling dimension* of the operator \mathcal{O}_n^* . An operator with scaling dimension $\gamma_n < 0$ is called *relevant*, because it becomes increasingly important as Λ decreases towards 0 and thus has a dramatic effect on the physics at low energies. An operator with scaling dimension $\gamma_n > 0$ is called *irrelevant*, because it decreases in importance as Λ decreases towards 0. An operator with scaling dimension $\gamma_n = 0$ is called *marginal*. The Hamiltonian density can be expanded around the fixed point in terms of the scaling operators:

$$\mathcal{H} = \mathcal{H}^* + \sum_{n=1}^{\infty} c_n(\Lambda) \mathcal{O}_n^*. \quad (43)$$

Once the scaling operators have been identified and their scaling dimensions γ_n determined, the model can be truncated to include only a finite number of terms in the Hamiltonian. A consistent truncation must include all the operators that are relevant and marginal. The behavior of the system near the fixed point can be described more accurately by including irrelevant operators. The accuracy of the description can be systematically improved by adding operators with increasing values of γ_n .

The simplest example of a renormalization group fixed point is the free theory with the Hamiltonian density $\mathcal{H}_{\text{free}}$ in Eq. (27). This fixed point is called the *trivial fixed point*. The forms of the scaling operators depend on the choice of ultraviolet cutoff or regularization. With a scale-invariant regularization

scheme, such as dimensional regularization, the scaling operators consist of terms that all have the same engineering dimensions. A scaling operator with N factors of ψ , N factors of ψ^\dagger , and D factors of ∇ has scaling dimension $3N + D - 5$. The 2-body interaction terms in Eq. (28) are irrelevant operators with scaling dimensions 1 and 3, respectively. The simplest 3-body interaction term $(\psi^\dagger)^3\psi^3$ is an irrelevant operator with scaling dimension 4. The successive truncation of the Hamiltonian to include operators with increasingly higher scaling dimension corresponds to a combination of the gradient expansion and an expansion in the number of particles.

The system of nonrelativistic particles with short-range interactions also has a nontrivial fixed point. In terms of the effective range expansion in Eq. (17), the fixed point corresponds to the limit in which the scattering length a is infinite and the effective range r_s and all higher coefficients in the expansion are 0. The dimensions of the scaling operators at the fixed point were deduced by Kaplan, Savage and Wise [7,8] and by van Kolck [9]. There is a relevant operator with scaling dimension -1 which if added to the fixed-point Hamiltonian gives a model with a finite scattering length. There are also irrelevant operators with scaling dimensions 1, 3, 5, \dots

4 Zero-Range Model

The simplest scattering model for ultracold atoms is the *Zero-Range Model*, whose only parameter is the scattering length a . The Zero-Range Model can be defined by the truncation of the effective range expansion in Eq. (17) after the constant term:

$$k \cot \delta_0(k) = -1/a. \quad (44)$$

The effective range and all the higher coefficients in the effective range expansion in Eq. (17) are exactly 0.

The Zero-Range Model provides a natural description for atoms with a large scattering length that arises from the accidental fine tuning of the depth of the interatomic potential. In such a case, the scattering length typically changes very slowly with the magnetic field B . Its dependence on B can be taken into account by allowing the parameter a in Eq. (44) to be a smooth function of B . The Zero-Range Model also provides a minimal description for atoms with a large scattering length that arises from any other mechanism. If that mechanism is a Feshbach resonance, the dependence of the scattering length a on B has the form given in Eq. (23).

4.1 Hamiltonian

The Zero-Range Model can be described by a quantum field theory with the single complex field ψ . The Hamiltonian density is the sum of the free term in Eq. (27) and the interaction term

$$\mathcal{H}_{\text{int}} = \frac{1}{4} \lambda_0 (\psi^\dagger \psi)^2. \quad (45)$$

The interaction term corresponds to a momentum-independent vertex with the Feynman rule $-i\lambda_0$. Such an interaction is singular, so the model requires an ultraviolet cutoff Λ on the momenta of virtual atoms.

The Zero-Range Model is renormalizable in the 2-body sector. As shown in Sec. 4.2, the bare coupling constant λ_0 in Eq. (45) can be adjusted as a function of Λ so that 2-body observables do not depend on Λ . The scattering length has the desired value a if the bare coupling constant is

$$\lambda_0(\Lambda) = \left(1 - \frac{2}{\pi} a \Lambda\right)^{-1} \frac{8\pi a}{m}. \quad (46)$$

This expression can be inverted to express the scattering length as a function of the bare coupling constant and the cutoff:

$$a = \frac{m}{8\pi} \left[\frac{1}{\lambda_0} + \frac{m}{4\pi^2} \Lambda \right]^{-1}. \quad (47)$$

The expression for the bare coupling constant in Eq. (46) provides a simple illustration of Wilsonian renormalization, which was discussed in Sec. 3.7. The operator $(\psi^\dagger \psi)^2$ in Eq. (45) has engineering dimension 6. The corresponding dimensionless coupling constant is therefore $\Lambda \lambda_0(\Lambda)$. This dimensionless coupling constant has fixed points for two values of the scattering length: $a = 0$ and $a = \pm\infty$. The trivial fixed point $a = 0$ corresponds to a noninteracting theory. For infinitesimal values of a , the dimensionless coupling constant is $\Lambda \lambda_0(\Lambda) \approx 8\pi a \Lambda / m$. Thus near the trivial fixed point, $(\psi^\dagger \psi)^2$ is an irrelevant operator with scaling dimension 1. The nontrivial fixed point $a = \pm\infty$ is commonly referred to as the *unitary limit*. At the fixed point, the dimensionless coupling constant is $\hat{\lambda}_0^* \approx -4\pi^2 / m$. For infinitesimal values of $1/a$, the deviation of the dimensionless coupling constant from its fixed-point value is $\Lambda \lambda_0(\Lambda) - \hat{\lambda}_0^* \approx -2\pi^3 / (ma\Lambda)$. Thus near the unitary fixed point, $(\psi^\dagger \psi)^2$ is a relevant operator with scaling dimension -1 .

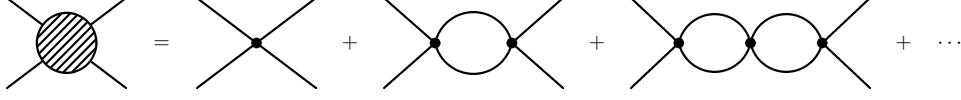


Fig. 3. The series of diagrams whose sum is the amputated connected Green's function for atom-atom scattering in a model with contact interactions only, such as the Zero-Range Model.

4.2 Green's function

The amputated connected Green's function for 2 atoms to evolve into 2 atoms can be calculated analytically by summing the series of diagrams shown in Fig. 3. Each vertex gives a factor of $-i\lambda_0$. Each loop gives the product of two propagators, which must be integrated over the momenta and energies of the virtual atoms. In the center-of-mass frame, the integral is

$$\begin{aligned} \int \frac{d\omega}{2\pi} \int \frac{d^3k}{(2\pi)^3} \frac{i}{\omega - k^2/(2m) + i\varepsilon} \frac{i}{E - \omega - k^2/(2m) + i\varepsilon} \\ = \int \frac{d^3k}{(2\pi)^3} \frac{i}{E - k^2/m + i\varepsilon}, \end{aligned} \quad (48)$$

where E is the total energy in that frame. The energy integral has been evaluated using contour integration. The remaining momentum integral is ultraviolet divergent. It can be regularized by imposing a momentum cutoff: $|\mathbf{k}| < \Lambda$. For each loop, there is also a symmetry factor of $\frac{1}{2}$. The resulting expression for the amplitude is

$$i\mathcal{A}(E) = -i\lambda_0 \sum_{n=0}^{\infty} \left[(-i\lambda_0) \frac{1}{2} \int \frac{d^3k}{(2\pi)^3} \frac{i}{E - k^2/m + i\varepsilon} \right]^n. \quad (49)$$

The amplitude depends on the total energy E of the two atoms in the center-of-mass frame, but not on the momenta of the incoming or outgoing atoms. The sum of the geometric series in Eq. (49) is

$$\mathcal{A}(E) = -\lambda_0 \left(1 - \frac{\lambda_0}{2} I_0(E) \right)^{-1}, \quad (50)$$

where the integral $I_0(E)$ is defined in Eq. (A.1). The expression for the integral is particularly simple if we take Λ to be so much larger than $(m|E|)^{1/2}$ that we can neglect terms that decrease as inverse powers of $\Lambda/(m|E|)^{1/2}$ as $\Lambda \rightarrow \infty$. The integral is given in the Appendix in Eq. (A.3). The resulting expression for the Green's function is

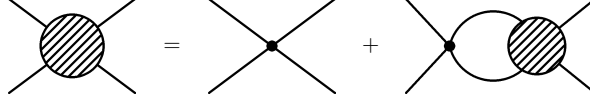


Fig. 4. The integral equation for the amputated connected Green's function for atom-atom scattering in a model with contact interactions only, such as the Zero-Range Model.

$$\mathcal{A}(E) = - \left[\frac{1}{\lambda_0} + \frac{m}{4\pi^2} \Lambda - \frac{m}{8\pi} \kappa \right]^{-1}, \quad (51)$$

where κ is proportional to the square root of the energy:

$$\kappa = (-mE - i\varepsilon)^{1/2}. \quad (52)$$

The amplitude in Eq. (51) can also be obtained by solving the Lippmann-Schwinger integral equation, which is represented diagrammatically in Fig. 4 and can be written

$$i\mathcal{A}(E) = -i\lambda_0 + (-i\lambda_0) \frac{1}{2} \int \frac{d^3k}{(2\pi)^3} \frac{i}{E - k^2/m + i\varepsilon} (i\mathcal{A}(E)). \quad (53)$$

Since $\mathcal{A}(E)$ does not depend on the momenta of the incoming or outgoing particles, this is just a linear equation for $\mathcal{A}(E)$ and its solution is Eq. (51).

The dependence of the amplitude in Eq. (51) on the ultraviolet cutoff can be eliminated by choosing the bare coupling constant $\lambda_0(\Lambda)$ to have the form in Eq. (46), where a is an arbitrary parameter with dimensions of length. The renormalized expression for the amplitude is then obtained by using Eq. (46) to eliminate λ_0 in favor of a :

$$\mathcal{A}(E) = -\frac{8\pi}{m} \frac{a}{1 - a\kappa}. \quad (54)$$

Since $\mathcal{A}(E)$ encodes all the physical 2-body observables, we conclude that the Zero-Range Model is renormalizable in the 2-body sector.

A simple way to reproduce the renormalized expression for $\mathcal{A}(E)$ in Eq. (54) is to use *dimensional regularization*, which automatically subtracts power ultraviolet divergences such as the linear term in Λ in Eq. (A.3). With this regularization scheme, the integral $I_0(E)$ is given simply by Eq. (A.6a). Since no renormalization is necessary in this case, we call the parameter λ instead of λ_0 . The amplitude in Eq. (50) then reduces to

$$\mathcal{A}(E) = - \left[\frac{1}{\lambda} - \frac{m}{8\pi} \kappa \right]^{-1}. \quad (55)$$

This agrees with Eq. (54) if we set $\lambda = 8\pi a/m$.

4.3 *T-matrix element*

The T-matrix element for atom-atom scattering with relative momentum k can be obtained from $\mathcal{A}(E)$ in Eq. (54) by setting E equal to the total kinetic energy $2(k^2/2m)$ of the two atoms:

$$\mathcal{T}(k) = -\frac{8\pi}{m} \frac{a}{1 + iak}. \quad (56)$$

By taking the low-energy limit $k \rightarrow 0$ and comparing with Eq. (14), we identify a as the scattering length. Comparing with Eq. (16), we obtain the simple equation for the phase shift in Eq. (44).

4.4 *Bound state*

The amplitude $\mathcal{A}(E)$ in Eq. (54) has a pole in the energy variable κ defined in Eq. (52). The pole is at $\kappa = 1/a$. If $a > 0$, this corresponds to a pole in the energy at $E = -1/(ma^2)$, which implies that there is a stable bound state with binding energy $1/(ma^2)$. This bound state is the *shallow dimer*, whose binding energy is given in Eq. (21). If $a < 0$, the pole at $\kappa = 1/a$ corresponds to pole at $E = -1/(ma^2)$ on the second sheet of the complex variable E . Such a pole corresponds to a virtual state.

4.5 *Optical Theorem*

If the energy E is real, the imaginary part of the amplitude in Eq. (54) is

$$\text{Im } \mathcal{A}(E) = \frac{(8\pi/m)a^2k}{1 + a^2k^2} \theta(E) + \frac{16\pi^2/m^2}{a} \delta(E + 1/(ma^2)) \theta(a). \quad (57)$$

The first term is nonzero for positive values of $E = k^2/m$. The second term, which contributes only if $a > 0$, is a delta function at the negative energy $-E_D$. Note that the expression for $\text{Im } \mathcal{A}(E)$ in Eq. (57) is positive definite, in accord with the Optical Theorem in Eq. (29). This implies that there are no negative-norm states in the 2-atom sector of the Zero-Range Model.

4.6 Three-body sector

In the 2-body sector, the Zero-Range Model is completely defined by a single parameter: the scattering length a . In the 3-body and higher sectors, this condition is not sufficient to specify the model completely because of the *Efimov effect* [10,11]. In the unitary limit $a \rightarrow \pm\infty$, there are infinitely-many arbitrarily-shallow trimers called *Efimov states* whose energies $-E_T^{(n)}$ have an accumulation point at the 3-atom threshold. For $a = \pm\infty$, the spectrum is

$$E_T^{(n)} = (e^{2\pi/s_0})^{n_*-n} \frac{\hbar^2 \kappa_*^2}{m}, \quad (58)$$

where n_* is an integer, κ_* has dimensions of momentum, and s_0 is the transcendental number that satisfies

$$s_0 \cosh \frac{\pi s_0}{2} = \frac{8}{\sqrt{3}} \sinh \frac{\pi s_0}{6}. \quad (59)$$

Its numerical value is $s_0 \approx 1.00624$. The spectrum in Eq. (58) defines a 3-body parameter κ_* that is independent of a . One can interpret $\hbar^2 \kappa_*^2/m$ as the approximate binding energy of the trimer labeled n_* . A different choice of n_* gives a value of κ_* that differs by an integer power of $e^{\pi/s_0} \approx 22.7$. The ratio of successive binding energies in Eq. (58) is $e^{2\pi/s_0} \approx 515.03$. This spectrum in Eq. (58) is consistent with an asymptotic discrete scaling symmetry with discrete scaling factor $e^{\pi/s_0} \approx 22.7$. The 3-body observables are uniquely determined only if one specifies both the scattering length a and the 3-body parameter κ_* . The 3-body parameter κ_* can be adjusted by adding a $(\psi^\dagger \psi)^3$ term to the Hamiltonian [12,13]. The renormalization of its coefficient is governed by a limit cycle instead of a fixed point [2]. Thus if the Zero-Range Model is extended to include a $(\psi^\dagger \psi)^3$ interaction term, it is renormalizable in the 3-atom sector.

It is an open question whether the Zero-Range Model is renormalizable in the 4-atom and higher sectors. One problem is that the spectrum of Efimov states in Eq. (58) is unbounded from below in the limit $\Lambda \rightarrow \infty$, where Λ is the ultraviolet cutoff. Thus there can be no stable 4-atom bound states in the Zero-Range Model, because they can decay into an Efimov state and an atom. In spite of this pathology of the model, it is still possible that low-energy observables in the 4-atom and higher sectors have well-defined universal limits as $\Lambda \rightarrow \infty$ that depend only on the parameters a and κ_* . There is numerical evidence that this is the case in the 4-atom sector [14,15].

5 Effective Range Model

The simplest generalization of the Zero-Range Model is the *Effective Range Model*, whose two parameters are the scattering length a and the effective range r_s . The Effective Range Model can be defined by the truncation of the effective range expansion in Eq. (17) after the k^2 term:

$$k \cot \delta_0(k) = -1/a + \frac{1}{2}r_s k^2. \quad (60)$$

All the higher coefficients in the effective range expansion are 0. The Effective Range Model provides a natural description for atoms that have a large scattering length and a large effective range because of a double fine-tuning. It can also describe atoms with a large scattering length and a natural effective range more accurately than the Zero-Range Model.

Phillips, Beane, and Cohen showed that the phase shift in Eq. (60) can be reproduced by a renormalizable local Hamiltonian quantum field theory with a single atom field only if the effective range r_s is negative [16]. This will be verified below in Sec. 5.3. In Sec. 8, we will show that the phase shift in Eq. (60) can also be reproduced by a renormalizable local Hamiltonian quantum field theory with an atom field and a molecular field, but again only if $r_s < 0$. In Sec. 6.3, we will show that the phase shift in Eq. (60) with either sign of r_s can be reproduced by a Lagrangian quantum field theory with a time-derivative interaction. However, if $r_s > 0$, the price that must be paid is a space of quantum states that includes negative-norm states.

5.1 Hamiltonian

The simplest Hamiltonian quantum field theory that gives a nonzero effective range has the two interaction terms in Eq. (28), which can also be expressed in the form

$$\mathcal{H}_{\text{int}} = \frac{1}{4}\lambda_0(\psi^\dagger\psi)^2 + \frac{1}{4}\rho_0\nabla(\psi^\dagger\psi) \cdot \nabla(\psi^\dagger\psi). \quad (61)$$

The second interaction term can be expressed in an alternative form using Eq. (37):

$$\mathcal{H}_{\text{int}} = \frac{1}{4}\lambda_0(\psi^2)^\dagger\psi^2 - \frac{1}{16}\rho_0 \left[(\psi^2)^\dagger(\psi\overleftrightarrow{\nabla}^2\psi) + (\psi\overleftrightarrow{\nabla}^2\psi)^\dagger\psi^2 \right]. \quad (62)$$

The difference between the Hamiltonian densities in Eqs. (61) and (62) is a total divergence, so it gives zero when integrated over all space to get the Hamiltonian. The elementary vertex for particles with momenta \mathbf{p}_1 and \mathbf{p}_2 to scatter into momenta \mathbf{p}'_1 and \mathbf{p}'_2 is

$$-i \left(\lambda_0 + \frac{1}{4} \rho_0 [(\mathbf{p}_1 - \mathbf{p}_2)^2 + (\mathbf{p}'_1 - \mathbf{p}'_2)^2] \right) = -i [\lambda_0 + \rho_0(k^2 + k'^2)], \quad (63)$$

where $k = \frac{1}{2}|\mathbf{p}_1 - \mathbf{p}_2|$ and $k' = \frac{1}{2}|\mathbf{p}'_1 - \mathbf{p}'_2|$ are the relative momenta in the initial and final states.

As shown by Phillips, Beane, and Cohen, the Effective Range Model is renormalizable in the 2-body sector provided the effective range r_s is negative [16]. The bare coupling constants λ_0 and ρ_0 in Eq. (62) can be adjusted as functions of the ultraviolet cutoff Λ so that 2-body Green's functions and 2-body observables have finite limits as $\Lambda \rightarrow \infty$. The intricate tuning that is required will be derived in Sec. 5.3:

$$\rho_0(\Lambda) \longrightarrow -\frac{12\pi^2}{m\Lambda^3} \left[1 \pm \left(\frac{-12}{\pi r_s \Lambda} \right)^{1/2} \left(1 - \frac{\pi}{2a\Lambda} + \frac{6}{\pi r_s \Lambda} + \dots \right) \right], \quad (64a)$$

$$\lambda_0(\Lambda) \longrightarrow \frac{m}{20\pi^2} \rho_0(\Lambda)^2 \Lambda^5 + \frac{48\pi}{m r_s \Lambda^2} \left(1 - \frac{\pi}{2a\Lambda} + \frac{12}{\pi r_s \Lambda} + \dots \right). \quad (64b)$$

Note that the dimensionless coupling constants $\Lambda\lambda_0$ and $\Lambda^3\rho_0$ approach finite limits as $\Lambda \rightarrow \infty$.

5.2 Green's function

The amputated connected Green's function for two atoms can be calculated analytically by solving the Lippmann-Schwinger integral equation represented diagrammatically in Fig. 4. This equation can be solved most easily by assuming that the amplitude can be expressed in the form

$$\mathcal{A}(E; k, k') = \mathcal{A}_0(E) + \mathcal{A}_1(E)(k^2 + k'^2) + \mathcal{A}_2(E)k^2k'^2. \quad (65)$$

The integral equation then reduces to a system of linear equations for the three functions $\mathcal{A}_0(E)$, $\mathcal{A}_1(E)$, and $\mathcal{A}_2(E)$ [16]. The final result for the amplitude can be expressed in the form

$$\mathcal{A}(E; k, k') = -\frac{N(E; k, k')}{D(E)}. \quad (66)$$

The numerator is a function of E , k , k' , and Λ :

$$\begin{aligned}
N(E; k, k') = & \left(\lambda_0 - \frac{m}{20\pi^2} \rho_0^2 \Lambda^5 \right) - 2\rho_0 \left(1 + \frac{m}{24\pi^2} \rho_0 \Lambda^3 \right) \kappa^2 \\
& + \rho_0 \left(1 + \frac{m}{12\pi^2} \rho_0 \Lambda^3 \right) (2\kappa^2 + k^2 + k'^2) \\
& - \frac{m}{4\pi^2} \rho_0^2 \left(\Lambda - \frac{\pi}{2} \kappa \right) (\kappa^2 + k^2) (\kappa^2 + k'^2), \tag{67}
\end{aligned}$$

where $\kappa = (-mE - i\varepsilon)^{1/2}$. The denominator is a function of E and Λ :

$$\begin{aligned}
D(E) = & \left(1 + \frac{m}{12\pi^2} \rho_0 \Lambda^3 \right)^2 + \frac{m}{4\pi^2} \left[\left(\lambda_0 - \frac{m}{20\pi^2} \rho_0^2 \Lambda^5 \right) \right. \\
& \left. - 2\rho_0 \left(1 + \frac{m}{24\pi^2} \rho_0 \Lambda^3 \right) \kappa^2 \right] \left(\Lambda - \frac{\pi}{2} \kappa \right). \tag{68}
\end{aligned}$$

Since the numerator is a linear combination of four independent functions of κ , k , and k' , the dependence of the amplitude $\mathcal{A}(E; k, k')$ on Λ cannot be completely eliminated simply by taking the two bare parameters λ_0 and ρ_0 to be functions of Λ . However, as shown by Phillips, Beane, and Cohen [16], if the bare parameters λ_0 and ρ_0 are tuned as in Eqs. (64), the ratio in Eq. (66) will have a finite limit as $\Lambda \rightarrow \infty$. The renormalized amplitude obtained by this limiting procedure has the form

$$\mathcal{A}(E) = -\frac{8\pi}{m} \frac{a}{1 + \frac{1}{2} r_s a \kappa^2 - a \kappa}. \tag{69}$$

It depends on the total energy E but not on the momenta k and k' .

5.3 *T-matrix element*

The T-matrix element for atom-atom scattering with relative momentum k can be obtained from $\mathcal{A}(E)$ in Eq. (69) by setting E equal to the total energy k^2/m of the two atoms:

$$\mathcal{T}(k) = -\frac{8\pi}{m} \frac{a}{1 - \frac{1}{2} r_s a k^2 + i a k}. \tag{70}$$

Comparing with Eq. (16), we obtain the equation for the phase shift in Eq. (60).

To drive the expressions for the tuning of the bare parameters in Eqs. (64), we start from the unrenormalized expression for the T-matrix element obtained by setting $k' = k$ and $\kappa = -ik$ in the Green's function $\mathcal{A}(E; k, k')$ given by Eqs. (66), (67), and (68):

$$\mathcal{T}(k) = - \left(\frac{[1 + (m/12\pi^2)\rho_0\Lambda^3]^2}{[\lambda_0 - (m/20\pi^2)\rho_0^2\Lambda^5] + 2\rho_0[1 + (m/24\pi^2)\rho_0\Lambda^3]k^2} + \frac{m}{4\pi^2}\Lambda + i\frac{m}{8\pi}k \right)^{-1}. \quad (71)$$

Expanding $\mathcal{T}(k)^{-1}$ in powers of k and comparing with the effective range expansion in Eq. (17), we find that the scattering length and the effective range are

$$a = \frac{m}{8\pi} \frac{1}{[1 + (m/12\pi^2)\rho_0\Lambda^3]^2 / [\lambda_0 - (m/20\pi^2)\rho_0^2\Lambda^5] + (m/4\pi^2)\Lambda}, \quad (72a)$$

$$r_s = \frac{32\pi}{m} \frac{\rho_0[1 + (m/12\pi^2)\rho_0\Lambda^3]^2[1 + (m/24\pi^2)\rho_0\Lambda^3]}{[\lambda_0 - (m/20\pi^2)\rho_0^2\Lambda^5]^2}. \quad (72b)$$

Using Eq. (72a) to eliminate λ_0 in favor of a , the expression for the effective range in Eq. (72b) becomes

$$r_s = \frac{2m}{\pi^3} \frac{\rho_0[1 + (m/24\pi^2)\rho_0\Lambda^3]}{[1 + (m/12\pi^2)\rho_0\Lambda^3]^2} \left[\Lambda - \frac{\pi}{2a} \right]^2. \quad (73)$$

One can show that for the right side of Eq. (73) to have a finite nonzero limit as $\Lambda \rightarrow \infty$, the quantity $1 + (m/12\pi^2)\rho_0\Lambda^3$ in the denominator must approach 0 as $\Lambda^{-1/2}$:

$$[1 + (m/12\pi^2)\rho_0\Lambda^3]^2 \longrightarrow -\frac{12}{\pi r_s \Lambda} \left(1 - \frac{\pi}{a\Lambda} + \frac{12}{\pi r_s \Lambda} + \dots \right). \quad (74)$$

This equation implies that the bare parameter ρ_0 must have the limiting behavior given in Eq. (64a).

If we insert the limiting expression in Eq. (74) into the expression for the scattering length in Eq. (72a), it reduces to

$$a = \frac{m}{8\pi} \left[\frac{-12/(\pi r_s \Lambda)}{\lambda_0 - (m/20\pi^2)\rho_0^2\Lambda^5} \left(1 - \frac{\pi}{a\Lambda} + \frac{12}{\pi r_s \Lambda} + \dots \right) + \frac{m}{4\pi^2}\Lambda \right]^{-1}. \quad (75)$$

This shows that the quantity $\lambda_0 - (m/20\pi^2)\rho_0^2\Lambda^5$ must approach 0 as Λ^{-2} :

$$\lambda_0 - \frac{m}{20\pi^2}\rho_0^2\Lambda^5 \longrightarrow \frac{48\pi}{mr_s\Lambda^2} \left(1 - \frac{\pi}{2a\Lambda} + \frac{12}{\pi r_s\Lambda} + \dots \right). \quad (76)$$

It also implies that the bare parameter λ_0 must have the limiting behavior given in Eq. (64b).

After inserting the limiting expressions in Eqs. (74) and (76), the T-matrix element in Eq. (71) reduces to

$$\mathcal{T}(k) = -\frac{8\pi}{m} \lim_{\Lambda \rightarrow \infty} \left[-\frac{2}{\pi}\Lambda \left(1 + \frac{\pi}{2a\Lambda} - \frac{\pi r_s k^2}{4\Lambda} \right)^{-1} + \frac{2}{\pi}\Lambda + ik \right]^{-1}. \quad (77)$$

Taking the limit $\Lambda \rightarrow \infty$, we recover the renormalized expression for the T-matrix element in Eq. (70).

Since the left side of Eq. (74) is positive definite, this equation implies that the effective range r_s in this model must be negative. This result was first derived by Phillips, Beane, and Cohen [16]. They showed that this conclusion is more general. The effective range must be negative for any model with a Hamiltonian that includes gradient interactions of arbitrarily high order. This result is consistent with a proof that the self-adjoint extension of the Hamiltonian with a delta-function potential to a 2-parameter Hamiltonian with scattering length a and effective range r_s can be made on a Hilbert space with positive definite norm only if $r_s < 0$ [17].

5.4 Bound states

The amplitude $\mathcal{A}(E)$ in Eq. (69) has two poles in the energy variable κ defined by Eq. (52). The values of κ at the poles satisfy a quadratic equation:

$$1 - a\kappa + \frac{1}{2}r_s a\kappa^2 = 0. \quad (78)$$

If there is a positive real root κ_i , there is a stable bound state with binding energy κ_i^2/m . If there is a negative real root κ_i , the pole corresponds to a virtual state. The quadratic polynomial in Eq. (78) has no real roots if $a/r_s < 2$. If $a/r_s > 2$, it has two real roots:

$$\kappa_{\pm} = \frac{1}{r_s} \left(1 \pm \sqrt{1 - 2r_s/a} \right). \quad (79)$$

The condition $a/r_s > 2$ requires a and r_s to either have opposite signs or to have the same signs and satisfy $|a| > 2|r_s|$. The root κ_- is positive if $a > 0$ and negative if $a < 0$. The root κ_+ is positive if $r_s > 0$ and negative if $r_s < 0$. Thus there can be 0, 1, or 2 stable bound states depending on the signs of a and r_s .

If $|a|$ is large compared to $|r_s|$, the approximate solutions are $\kappa_- \approx 1/a$ and $\kappa_+ \approx 2/r_s$. The solution κ_- corresponds to the shallow dimer if $a > 0$ and to a shallow virtual state if $a < 0$. If $r_s < 0$, as required by the renormalizability of the Effective Range Model, the solution κ_+ corresponds to a virtual state. If $r_s > 0$ was allowed, the solution κ_+ would correspond to a stable deeply-bound state.

5.5 Optical theorem

If the energy E is real and $a/r_s > 2$, the imaginary part of the amplitude in Eq. (69) is

$$\begin{aligned} \text{Im } \mathcal{A}(E) = & \frac{(8\pi/m)a^2k}{(1 - \frac{1}{2}r_s a k^2)^2 + a^2 k^2} \theta(E) \\ & + \frac{16\pi^2/m^2}{\sqrt{1 - 2r_s/a}} \left[\kappa_- \delta(E + \kappa_-^2/m) \theta(a) - \kappa_+ \delta(E + \kappa_+^2/m) \theta(r_s) \right]. \end{aligned} \quad (80)$$

The first term is nonzero for positive values of $E = k^2/m$. This is the only term if $a/r_s < 2$. If $a/r_s > 2$, there can also be delta function contributions at negative values of E . There is a delta function term with a positive coefficient if $a > 0$ and another delta function term with a negative coefficient if $r_s > 0$. Thus if $r_s > 0$, the Optical Theorem includes a negative-definite term as in Eq. (34). The bound state associated with this term can be interpreted as a state with negative norm. The condition $r_s < 0$ for the absence of negative-norm states coincides with the condition for the renormalizability of the Effective Range Model. If there is a large scattering length $|a| \gg r_s$, the negative-norm state corresponds to a deeply-bound state.

6 Other Single-Channel models

In this sector, we describe briefly other scattering models that can be formulated as local quantum field theories with a single quantum field ψ .

6.1 Higher-gradient interactions

One straightforward generalization of the Effective Range Model is to include higher gradient terms in the interaction Hamiltonian. There are two independent terms with four gradients that give only S -wave scattering:

$$\begin{aligned} \Delta\mathcal{H}_{\text{int}} = & \mu_0 \left(\psi \overleftrightarrow{\nabla}^2 \psi \right)^\dagger \left(\psi \overleftrightarrow{\nabla}^2 \psi \right) \\ & + \mu'_0 \left[(\psi^2)^\dagger \left(\psi \overleftrightarrow{\nabla}^2 \overleftrightarrow{\nabla}^2 \psi \right) + \left(\psi \overleftrightarrow{\nabla}^2 \overleftrightarrow{\nabla}^2 \psi \right)^\dagger \psi^2 \right]. \end{aligned} \quad (81)$$

The model whose Hamiltonian is the sum of $\mathcal{H}_{\text{free}}$ in Eq. (27), \mathcal{H}_{int} in Eq. (61), and $\Delta\mathcal{H}_{\text{int}}$ in Eq. (81) has four bare parameters that can depend on the ultraviolet cutoff. If this model is renormalizable, one might expect it to be able to reproduce additional terms in the effective range expansion of the S -wave phase shift in Eq. (17) beyond the two terms that are shown. Such a model is not of much practical use for atoms, because the $1/r^6$ tail of the van der Waals potential implies that $k \cot \delta_0(k)$ has an expansion in powers of k^2 only to order k^2 .

In Ref. [18], the Green's function $\mathcal{A}(E; k, k')$ for this model with an ultraviolet cutoff Λ was obtained by solving the Lippmann-Schwinger integral equation shown diagrammatically in Fig. 4. The authors showed that the dependence of the T-matrix element on the ultraviolet cutoff could not be removed simply by choosing the bare parameters to be functions of Λ , as in the Zero-Range Model in Sec. 4. However, they did not investigate whether the model is renormalizable in the sense of having a nontrivial limit as $\Lambda \rightarrow \infty$, as in the Effective Range Model in Sec. 5. Since the Effective Range Model is the special case $\mu_0 = \mu'_0 = 0$, it is clear that the four bare parameters can be chosen as functions of Λ so that the phase shift in the limit $\Lambda \rightarrow \infty$ is Eq. (60) with $r_s < 0$. It is not known whether a more general phase shift can be obtained by taking such a limit.

6.2 Dimensional regularization

If there is a consistent way to renormalize a quantum field theory, one can often obtain the final result more simply by using dimensional regularization. In this regularization method, ultraviolet-divergent integrals over a 3-dimensional momentum are generalized to a variable number of dimension d , evaluated in a range of d for which they converge, and then analytically continued to $d = 3$. This regularization prescription treats power divergences very differently from logarithmic divergences. Power-divergent integrals are those that diverge as

a positive power Λ^p with a momentum cutoff Λ . Logarithmically-divergent integrals are those that diverge as $\log \Lambda$ as $\Lambda \rightarrow \infty$. Dimensional regularization sets power divergence to 0, while logarithmic divergences appear as poles in $d - 3$.

In the Effective Range Model, which is defined by the interaction Hamiltonian in Eq. (61), the only ultraviolet divergences that appear are power divergences Λ^p with $p = 1, 3, 5$. Dimensional regularization sets these divergences to 0. Thus the Green's function $\mathcal{A}(E; k, k')$ with dimensional regularization can be obtained from the results in Eqs. (66), (67), and (68) with a momentum cutoff simply by setting $\Lambda = 0$. The resulting expression is

$$\mathcal{A}(E; k, k') = -\frac{\lambda + \rho(k^2 + k'^2) + (m/8\pi)\rho^2\kappa(\kappa^2 + k^2)(\kappa^2 + k'^2)}{1 - (m/8\pi)(\lambda - 2\rho\kappa^2)\kappa}. \quad (82)$$

Since no renormalization is required, we have replaced the bare parameters λ_0 and ρ_0 by λ and ρ . The T-matrix element $\mathcal{T}(k)$ for atom-atom scattering can be obtained from the amplitude $\mathcal{A}(E; k, k')$ in Eq. (82) by setting $k' = k$ and $\kappa = -ik$:

$$\mathcal{T}(k) = -\frac{1}{1/(\lambda + 2\rho k^2) + i(m/8\pi)k}. \quad (83)$$

Expanding $\mathcal{T}(k)^{-1}$ in powers of k and comparing with the effective range expansion in Eq. (17), we find that the parameters λ and ρ are related in a simple way to the scattering length and the effective range: $\lambda = 8\pi a/m$, $\rho = 2\pi a^2 r_s/m$. If λ and ρ are eliminated in favor of a and r_s , the T-matrix element in Eq. (83) reduces to

$$\mathcal{T}(k) = -\frac{8\pi}{m} \frac{a}{1/(1 + \frac{1}{2}r_s a k^2) + iak}. \quad (84)$$

This result corresponds to the S -wave phase shift

$$k \cot \delta_0(k) = -\frac{1}{a \left(1 + \frac{1}{2}r_s a k^2\right)}. \quad (85)$$

The phase shift in Eq. (85) obtained using dimensional regularization has a different dependence on k from the phase shift in Eq. (60) obtained using a momentum cutoff regularization. Renormalization of the Effective Range Model using a momentum cutoff requires the constraint $r_s < 0$. There is no apparent constraint on r_s if we use dimensional regularization. This puzzle

was first pointed out in Ref. [16]. The fact that dimensional regularization of the Effective Range Model gives the phase shift in Eq. (85) suggests that there might be a more elaborate model with a momentum cutoff that gives this phase shift. However, the results of Ref. [16] imply that such a model cannot be a Hamiltonian quantum field theory.

6.3 Time-derivative interactions

Interactions that involve time derivatives are not allowed in a conventional Hamiltonian quantum field theory. However, they can be easily included in the Lagrangian approach. We will consider only the simplest Lagrangian model with a time-derivative interaction and show that it is equivalent to the Effective Range Model.

The Lagrangian density for a free atom is given in Eq. (32). The interaction term in the Lagrangian density for the Zero-Range Model is $\mathcal{L}_{\text{int}} = -\mathcal{H}_{\text{int}}$, where \mathcal{H}_{int} is given in Eq. (45). The simplest generalization of the Zero-Range Model that includes a time-derivative interaction is a model whose interaction term is

$$\mathcal{L}_{\text{int}} = -\frac{1}{4}(\psi^2)^\dagger \left(\lambda_0 - m\lambda'_0 \left(i\frac{\partial}{\partial t} + \frac{\nabla^2}{4m} \right) \right) \psi^2. \quad (86)$$

The combination of time and space derivatives acting on ψ^2 is Galilean invariant.

The diagrammatic analysis of the model whose Lagrangian is the sum of Eqs. (32) and (86) is identical to that in the Zero-Range Model except that the interaction vertex depends on the total energy E of the interacting atoms in their center-of-mass frame. The amplitude in this model can be obtained from the unrenormalized Green's function for the Zero-Range Model in Eq. (51) simply by the substitution $\lambda_0 \rightarrow \lambda_0 + \lambda'_0 \kappa^2$, where $\kappa = (-mE - i\epsilon)^{1/2}$. The resulting expression for the Green's function is

$$\mathcal{A}(E) = - \left[\frac{1}{\lambda_0 + \lambda'_0 \kappa^2} + \frac{m}{4\pi^2} \Lambda - \frac{m}{8\pi} \kappa \right]^{-1}. \quad (87)$$

We obtain the T -matrix element $\mathcal{T}(k)$ by setting $\kappa = -ik$. By using the expression for $\mathcal{T}(k)$ in Eq. (16) and the expression for $k \cot \delta_0(k)$ in Eq. (17), we can determine the scattering length and effective range:

$$\frac{1}{a} = \frac{8\pi}{m} \left(\frac{1}{\lambda_0} + \frac{m}{4\pi^2} \Lambda \right), \quad (88a)$$

$$r_s = -\frac{16\pi}{m} \frac{\lambda'_0}{\lambda_0^2}. \quad (88b)$$

By inverting these equations, we can determine how the bare parameters λ_0 and λ'_0 must be tuned as functions of the cutoff Λ in order to keep a and r_s fixed:

$$\lambda_0(\Lambda) = \left(1 - \frac{2}{\pi} a \Lambda \right)^{-1} \frac{8\pi a}{m}, \quad (89a)$$

$$\lambda'_0(\Lambda) = -r_s \frac{4\pi a^2}{m} \left(1 - \frac{2}{\pi} a \Lambda \right)^{-2}. \quad (89b)$$

Inserting these expressions into Eq. (87) and taking the limit $\Lambda \rightarrow \infty$, we obtain the renormalized amplitude:

$$\mathcal{A}(E) = -\frac{8\pi}{m} \left[\frac{1}{a} + \frac{1}{2} r_s \kappa^2 - \kappa \right]^{-1}. \quad (90)$$

This is identical to the renormalized amplitude for the Effective Range Model in Eq. (69). Since all 2-body observables can be obtained from the Green's functions, we conclude that the Lagrangian field theory with the time-derivative interaction in Eq. (86) is equivalent to the Effective Range Model, at least in the 2-body sector.

6.4 Wilsonian renormalization

The Wilsonian approach to renormalization requires finding a fixed-point Hamiltonian \mathcal{H}^* together with scaling operators \mathcal{O}_n^* and their scaling dimensions γ_n . The Hamiltonian can then be expanded around the fixed point as in Eq. (43). The Wilsonian approach can also be applied to the larger space of Lagrangian quantum field theories. In this case, there is a similar expansion around a fixed-point Lagrangian \mathcal{L}^* .

In a remarkable paper, Birse, McGovern, and Richardson carried out a complete Wilsonian analysis of 2-body S-wave interactions [20]. In a Lagrangian quantum field theory, the general S-wave 2-body operator can be expressed in terms of a potential $V(p, k, k', \Lambda)$ that depends on the total energy $E = p^2/m$, the squares k^2 and k'^2 of the initial and final momenta, and the ultraviolet cutoff Λ . The requirement that the solution $\mathcal{A}(p, k, k')$ to the Lippmann-Schwinger integral equation be independent of the ultraviolet cutoff Λ gives renormalization group flow equations on the infinite-dimensional space of potentials. The

trivial fixed point is $V = 0$. There is also a nontrivial fixed point corresponding to the unitary limit of infinite scattering length:¹

$$V^*(p, \Lambda) = -\frac{4\pi^2}{m} \left[\Lambda - \frac{p}{2} \log \frac{\Lambda + p}{\Lambda - p} \right]^{-1}. \quad (91)$$

This can be expanded as a power series in p^2 , so it corresponds to an interaction term with arbitrarily high-order time derivatives. A system infinitesimally close to the fixed point has a potential of the form $V^*(p, \Lambda) + v(p, k, k', \Lambda)$. The authors of Ref. [20] found all the scaling operators $v(p, k, k', \Lambda)$. The scaling operators $v(p, \Lambda)$ that depend only on the energy variable p have the scaling dimensions $-1, 1, 3, 5, \dots$ that were deduced in Refs. [7,8,9]. There are also scaling operators $v(p, k, k', \Lambda)$ that have nontrivial dependence on the momentum variables k and k' . They have scaling dimensions $2, 4, 5, 6, \dots$. They may correspond to redundant operators in the Lagrangian formulation that have no counterparts in a Hamiltonian formulation and do not affect physical observables.

Harada and Kubo and collaborators have applied the Wilsonian renormalization approach to Lagrangian field theories that are truncated in the derivative expansion [21,22,23]. In Refs. [21,22] they considered the 3-parameter Lagrangian consisting of the free term in Eq. (32), the two interaction terms of the Effective Range Model in Eq. (62), and the time-derivative interaction in Eq. (86). This corresponds to a potential of the form

$$V(p, k, k', \Lambda) = \lambda_0(\Lambda) + \rho_0(\Lambda)(k^2 + k'^2) - \lambda'_0(\Lambda)p^2. \quad (92)$$

By demanding that the solution to the Lippmann-Schwinger integral equation have a cutoff-independent expansion to first order in p^2 , k^2 , and k'^2 , they obtained renormalization group flow equations for the coupling constants $\lambda_0(\Lambda)$, $\rho_0(\Lambda)$, and λ'_0 . These equations have 3 fixed points: the trivial fixed point, the nontrivial fixed point, and an unphysical fixed point that gives complex scaling dimensions. Near the nontrivial fixed point, there is a relevant operator with scaling dimension -1 and two irrelevant operators with scaling dimensions 1 and 2 . In Ref. [23], the analysis was extended to the next order in the derivative expansion, where there are 8 coupling constants. They found three fixed points, two fixed lines, and a fixed surface. One of the fixed points was identified as the nontrivial fixed point associated with infinite scattering length.

¹ This differs from the expression in Ref. [20] by a factor of 2 associated with identical particles.

7 Two-Channel Model

A scattering model can describe multiple spin states of an atom. A minimal model has two spin states, including the one of primary interest. In general, there are 3 scattering channels corresponding to both atoms in the lower state, both atoms in the upper state, and atoms in both states. We consider the simple case of momentum-independent interactions between the atoms, as in the Zero-Range Model. We further simplify the problem by assuming that there is nontrivial scattering only in the two channels in which both atoms are in the same spin state. We will refer to this model as the *Two-Channel Model*. If the energies of atoms at rest in the two spin states are 0 and $\nu/2$, the scattering thresholds are 0 and ν . We choose $\nu > 0$ and we take the spin state of primary interest to be the one that is lower in energy. The parameters of the Two-Channel Model can be defined by specifying the S-wave phase shift in the lower spin channel to be

$$k \cot \delta_0(k) = -\frac{1}{a_{11}} - \frac{1}{a_{12}^2} \left[-1/a_{22} + \sqrt{m\nu - k^2} \right]^{-1}. \quad (93)$$

In addition to the energy gap ν , there are three interaction parameters with dimensions of length: a_{11} , a_{12} , and a_{22} . The interaction parameters are defined in such a way that the two channels decouple in the limit $a_{12} \rightarrow \pm\infty$. In this limit, a_{11} and a_{22} reduce to the scattering lengths for the two independent channels.

The scattering length and the effective range for the lower spin channel are

$$a = \left(\frac{1}{a_{11}} + \frac{1}{a_{12}^2} \left[\sqrt{m\nu} - 1/a_{22} \right]^{-1} \right)^{-1}, \quad (94a)$$

$$r_s = -\frac{1}{a_{12}^2 \sqrt{m\nu}} \left[\sqrt{m\nu} - 1/a_{22} \right]^{-2}. \quad (94b)$$

Note that the effective range r_s is negative definite. There are various ways to tune the parameters to get a large scattering length a . If $a_{11} < a_{12}^2/a_{22}$, a large scattering length can be obtained by tuning the energy gap ν to near the critical value $(1/a_{22} - a_{11}/a_{12}^2)^2/m$. At ν approaches the critical value, the effective range approaches $r_s \rightarrow a_{22}a_{12}^4/[a_{11}^2(a_{11}a_{22} - a_{12}^2)]$. A large scattering length can also be obtained by tuning the interaction parameter a_{11} to the critical value $-a_{12}^2[\sqrt{m\nu} - 1/a_{22}]$.

A renormalizable Hamiltonian quantum field theory for a Two-Channel Model with two distinguishable particles with unequal masses was constructed by Cohen, Gelman, and van Kolck [24]. An essentially equivalent model has been

used to describe the effects of $\Delta\Delta$ states on the two-nucleon system [25]. In Sec. 7.6, we generalize the Two-Channel Model to one with N scattering channels.

7.1 Hamiltonian

The Two-Channel Model can be formulated as a quantum field theory with two complex fields ψ and ψ_2 . The Hamiltonian density for the Two-Channel Model is the sum of a free term and an interaction term:

$$\mathcal{H}_{\text{free}} = \frac{1}{2m} \nabla \psi^\dagger \cdot \nabla \psi + \frac{1}{2m} \nabla \psi_2^\dagger \cdot \nabla \psi_2 + \frac{1}{2} \nu \psi_2^\dagger \psi_2, \quad (95a)$$

$$\mathcal{H}_{\text{int}} = \frac{1}{4} \lambda_{0,11} (\psi^\dagger \psi)^2 + \frac{1}{4} \lambda_{0,12} [(\psi^\dagger \psi_2)^2 + (\psi_2^\dagger \psi)^2] + \frac{1}{4} \lambda_{0,22} (\psi_2^\dagger \psi_2)^2. \quad (95b)$$

The Two-Channel Model is renormalizable in the 2-atom sector. The relations between the physical parameters a_{ij} and bare parameters $\lambda_{0,ij}$ are

$$\frac{1}{a_{11}} = \frac{8\pi}{m} \frac{\lambda_{0,22}}{\lambda_{0,11} \lambda_{0,22} - \lambda_{0,12}^2} + \frac{2}{\pi} \Lambda, \quad (96a)$$

$$\frac{1}{a_{12}} = -\frac{8\pi}{m} \frac{\lambda_{0,12}}{\lambda_{0,11} \lambda_{0,22} - \lambda_{0,12}^2}, \quad (96b)$$

$$\frac{1}{a_{22}} = \frac{8\pi}{m} \frac{\lambda_{0,11}}{\lambda_{0,11} \lambda_{0,22} - \lambda_{0,12}^2} + \frac{2}{\pi} \Lambda. \quad (96c)$$

These equations can be expressed more compactly in the form

$$\frac{1}{a_{mn}} = \frac{8\pi}{m} (\lambda_0^{-1})_{mn} + \frac{2}{\pi} \Lambda \delta_{mn}, \quad (97)$$

where λ_0^{-1} is the inverse of the matrix λ_0 of coefficients $\lambda_{0,ij}$.

Renormalization invariants are functions of the bare parameters that are equal to the same functions of the corresponding renormalized parameters independent of the value of the ultraviolet cutoff. Parameters that require no renormalization, such as the energy gap ν , are renormalization invariants. An alternative choice for the remaining parameters of the Two-Channel Model are the entries λ_{mn} of the matrix λ whose inverse has the entries

$$(\lambda^{-1})_{mn} = \frac{m}{8\pi a_{mn}}. \quad (98)$$

With this choice of renormalized parameters, the traceless components of the matrices λ^{-1} and λ_0^{-1} are renormalization invariants:

$$(\lambda^{-1})_{11} - (\lambda^{-1})_{22} = (\lambda_0^{-1})_{11} - (\lambda_0^{-1})_{22}, \quad (99a)$$

$$(\lambda^{-1})_{12} = (\lambda_0^{-1})_{12}. \quad (99b)$$

If we take the three independent interaction parameters to be these two renormalization invariants and $\text{tr}(\lambda_0^{-1})$, the only bare parameter that must depend on the ultraviolet cutoff is $\text{tr}(\lambda_0^{-1})$.

7.2 Green's function

The amputated connected Green's function $\mathcal{A}(E)$ for the Two-Channel Model is a 2×2 matrix that depends on the total energy E in the center-of-mass frame. The inverse of the matrix $\mathcal{A}(E)$ can be calculated analytically by solving the coupled system of integral equations represented diagrammatically in Fig. 4:

$$A(E)^{-1} = \begin{pmatrix} -(\lambda_0^{-1})_{11} - (m/4\pi^2)(\Lambda - \pi\kappa/2) & -(\lambda_0^{-1})_{12} \\ -(\lambda_0^{-1})_{12} & -(\lambda_0^{-1})_{22} - (m/4\pi^2)(\Lambda - \pi\sqrt{m\nu + \kappa^2}/2) \end{pmatrix}, \quad (100)$$

where $\kappa = (-mE - i\varepsilon)^{1/2}$. Inserting the relations in Eq. (97) between the physical parameters a_{ij} and the bare parameters $\lambda_{0,ij}$, the dependence on the ultraviolet cutoff Λ disappears and the inverse matrix reduces to

$$\mathcal{A}(E)^{-1} = \frac{m}{8\pi} \begin{pmatrix} -1/a_{11} + \kappa & -1/a_{12} \\ -1/a_{12} & -1/a_{22} + \sqrt{m\nu + \kappa^2} \end{pmatrix}. \quad (101)$$

The square roots are defined for negative real arguments by the $i\varepsilon$ prescription in the definition of κ in Eq. (52). The explicit expression for the entries of this matrix are

$$\mathcal{A}_{11}(E) = \frac{8\pi}{m} \left(-\frac{1}{a_{11}} + \kappa - \frac{1}{a_{12}^2} \left[-\frac{1}{a_{22}} + \sqrt{m\nu + \kappa^2} \right]^{-1} \right)^{-1}, \quad (102a)$$

$$\mathcal{A}_{12}(E) = \frac{8\pi}{m} \left(-\frac{1}{a_{12}} + a_{12} \left[-\frac{1}{a_{11}} + \kappa \right] \left[-\frac{1}{a_{22}} + \sqrt{m\nu + \kappa^2} \right] \right)^{-1}, \quad (102b)$$

$$\mathcal{A}_{22}(E) = \frac{8\pi}{m} \left(-\frac{1}{a_{22}} + \sqrt{m\nu + \kappa^2} - \frac{1}{a_{12}^2} \left[-\frac{1}{a_{11}} + \kappa \right]^{-1} \right)^{-1}. \quad (102c)$$

These expressions agree with the results of Ref. [24] except for a factor of two associated with identical particles.²

7.3 *T-matrix element*

The T-matrix element for the elastic scattering of atoms in the first channel with relative momentum k is obtained by evaluating $\mathcal{A}_{11}(E)$ in Eq. (102a) at the total energy $E = k^2/m$:

$$\mathcal{T}_{11}(k) = \frac{8\pi}{m} \left(-\frac{1}{a_{11}} - ik - \frac{1}{a_{12}^2} \left[-\frac{1}{a_{22}} + \sqrt{m\nu - k^2} \right]^{-1} \right)^{-1}. \quad (103)$$

Comparing with Eq. (16), we obtain the equation for the phase shift in Eq. (93).

7.4 *Bound states*

The three entries of the matrix $\mathcal{A}(E)$ given by Eq. (102) all have poles at the same values of the energy variable κ . The values of κ at the poles satisfy the equation

$$\kappa = \frac{1}{a_{11}} + \frac{1}{a_{12}^2} \left[-\frac{1}{a_{22}} + \sqrt{m\nu + \kappa^2} \right]^{-1}. \quad (104)$$

By solving for the square root and then squaring both sides of the equation, one can show that the roots of Eq. (104) are also roots of a quartic polynomial. If the root κ_i is real and positive, there is a stable bound state below the scattering threshold for the first channel with binding energy κ_i^2/m . If $\sqrt{m\nu} > 1/a_{22}$, Eq. (104) can have 0 or 1 positive real roots. If $a_{22} > 0$ and $\sqrt{m\nu} < 1/a_{22}$, Eq. (104) can have 1 or 2 positive real roots. Thus the number of stable diatomic molecules can be 0, 1, or 2.

If the scattering length a is made large by tuning ν to near its critical value, Eq. (104) will have one small root $\kappa \approx 1/a$. If $a > 0$, the corresponding bound state is the shallow dimer. The remaining roots of Eq. (104) satisfy $|\kappa| \gg 1/|a|$. As $a \rightarrow \pm\infty$, these large roots approach solutions to a cubic equation:

$$\kappa^3 - \frac{2}{a_{11}}\kappa^2 + \left(\frac{1}{a_{11}^2} - \frac{2a_{11}}{a_{12}^2 a_{22}} + \frac{a_{11}^2}{a_{12}^4} \right) \kappa + \frac{2}{a_{12}^2} \left(\frac{1}{a_{22}} - \frac{a_{11}}{a_{12}^2} \right) \approx 0. \quad (105)$$

² There is an error in the component $\mathcal{A}_{22}(E)$ in Ref. [24], but it vanishes when the masses of the two particles are set equal.

Since this cubic equation was derived by squaring a square root, some of its roots may not correspond to roots of Eq. (104). If $a_{11} < 0$, the limiting form of Eq. (104) has no large positive real roots. If $a_{11} > 0$, it has one large positive real root. Thus the number of stable deeply-bound diatomic molecules is either 0 or 1.

7.5 Optical theorem

If the energy E is real, the imaginary part of the amplitude in Eq. (102a) is

$$\begin{aligned} \text{Im } \mathcal{A}_{11}(E) = & \frac{8\pi}{m} \left| -\frac{1}{a_{11}} - ik - \frac{1}{a_{12}^2} \left[-\frac{1}{a_{22}} + \sqrt{m\nu - k^2 - i\varepsilon} \right]^{-1} \right|^{-2} \\ & \times \left(k + \frac{\sqrt{k^2 - m\nu}/a_{12}^2 \theta(E - \nu)}{k^2 - m\nu + 1/a_{22}^2} \right) \theta(E) \\ & + \frac{16\pi^2}{m^2} \sum_i \kappa_i \left[1 + \frac{a_{12}^2 (\kappa_i - 1/a_{11})^2 \kappa_i}{\sqrt{m\nu + \kappa_i^2}} \right]^{-1} \delta(E + \kappa_i^2/m) \theta(\kappa_i), \end{aligned} \quad (106)$$

where the sum in the last term is over the 0, 1, or 2 positive real roots κ_i of Eq. (104). The expression for $\text{Im } \mathcal{A}_{11}(E)$ is positive definite, in accord with the Optical Theorem in Eq. (29). This is consistent with the absence of negative-norm states in the 2-atom sector of the Two-Channel Model.

7.6 Multi-channel models

The Two-Channel Model can be generalized to one with N spin states with nontrivial scattering only between pairs of atoms in the same spin state. We refer to this model as the *N-Channel model*. It has $\frac{1}{2}(N^2 + 3N - 2)$ parameters: the $N - 1$ energy gaps ν_n between the lowest 2-atom threshold ($\nu_1 \equiv 0$) and the n^{th} 2-atom threshold and $\frac{1}{2}N(N + 1)$ interaction parameters a_{mn} with dimensions of length. The parameters in the *N-Channel model* can be defined by specifying the S-wave phase shift to be

$$k \cot \delta_0(k) = -\frac{1}{a_{11}} - \frac{1}{C_{11}(k^2)} \sum_{n=2}^N \frac{C_{1n}(k^2)}{a_{1n}}, \quad (107)$$

where $C_{1n}(k^2)$ is the $1n$ cofactor of the $N \times N$ matrix whose mn entry is $(m/8\pi)(-1/a_{mn} + \sqrt{m\nu_n - k^2} \delta_{mn})$. The scattering length and the effective

range are obtained from the low-momentum expansion of Eq. (107):

$$a = \left(\frac{1}{a_{11}} + \frac{1}{C_{11}(0)} \sum_{n=2}^N \frac{C_{1n}(0)}{a_{1n}} \right)^{-1}, \quad (108a)$$

$$r_s = -2 \sum_{n=2}^N \frac{C_{11}(0)C'_{1n}(0) - C'_{11}(0)C_{1n}(0)}{a_{1n} C_{11}^2(0)}, \quad (108b)$$

where $C'_{1n}(k^2) = (d/dk^2)C_{1n}(k^2)$.

The N -Channel model can be formulated as a quantum field theory with N complex fields ψ_n , $n = 1, \dots, N$. The Hamiltonian density for the N -Channel model is the sum of a free term and an interaction term:

$$\mathcal{H}_{\text{free}} = \sum_{n=1}^N \left[\frac{1}{2m} \nabla \psi_n^\dagger \cdot \nabla \psi_n + \frac{1}{2} \nu_n \psi_n^\dagger \psi_n \right], \quad (109a)$$

$$\mathcal{H}_{\text{int}} = \frac{1}{4} \sum_{m=1}^N \sum_{n=1}^N \lambda_{0,mn} (\psi_m^\dagger \psi_n)^2. \quad (109b)$$

Note that $\nu_1 = 0$ by definition. The N -Channel model is renormalizable in the 2-atom sector. The energy gaps ν_n require no renormalization. The relations between the physical interaction parameters a_{mn} and the bare coupling constants $\lambda_{0,mn}(\Lambda)$ are

$$\frac{1}{a_{mn}} = \frac{8\pi}{m} \left(\lambda_0^{-1} \right)_{mn} + \frac{2}{\pi} \Lambda \delta_{mn}. \quad (110)$$

The amputated connected Green's function $\mathcal{A}(E)$ for this coupled-channel system is a $N \times N$ matrix that depends on the total energy E in the center-of-mass frame. The inverse matrix $\mathcal{A}(E)^{-1}$ can be obtained analytically by solving the coupled-channel integral equations represented diagrammatically in Fig. 4. After the renormalization using Eq. (110), the mn entry of the inverse matrix reduces to

$$(\mathcal{A}(E)^{-1})_{mn} = \frac{m}{8\pi} \left[-\frac{1}{a_{mn}} + \sqrt{m\nu_m + \kappa^2} \delta_{mn} \right], \quad (111)$$

where $\kappa = (-mE - i\varepsilon)^{1/2}$. This inverse matrix can be inverted by using the identity

$$\mathcal{A}_{mn}(E) = \frac{C_{nm}(-\kappa^2)}{\det(\mathcal{A}(E)^{-1})}, \quad (112)$$

where $C_{nm}(-\kappa^2)$ is the nm cofactor of the matrix $\mathcal{A}(E)^{-1}$ given in Eq. (111). Since the determinant is the sum of the products of the entries in any row (or column) and their cofactors, the mn entry of the matrix $\mathcal{A}(E)$ reduces to

$$\mathcal{A}_{mn}(E) = \frac{8\pi}{m} \left[-\frac{1}{C_{nm}(mE)} \sum_{l=1}^N \frac{C_{nl}(mE)}{a_{nl}} + \sqrt{m\nu_n + \kappa^2} \frac{C_{nn}(mE)}{C_{nm}(mE)} \right]^{-1}. \quad (113)$$

The T-matrix element for elastic scattering in the first channel is obtained by evaluating the expression for $\mathcal{A}_{11}(E)$ given by Eq. (113) at the energy $E = k^2/m$:

$$\mathcal{T}_{11}(k) = \frac{8\pi}{m} \left[-\frac{1}{a_{11}} - ik - \frac{1}{C_{11}(k^2)} \sum_{n=2}^N \frac{C_{1n}(k^2)}{a_{1n}} \right]^{-1}. \quad (114)$$

This T-matrix element gives the S-wave phase shift for the N -Channel model in Eq. (107).

8 Resonance Model

The basic degrees of freedom in a scattering model can include molecular states as well as atoms. A minimal model has a single diatomic molecule that couples to a pair of atoms in the spin state of interest. We consider the simplest case of a momentum-independent interaction between the atoms and a momentum-independent coupling of the molecule to a pair of atoms. We treat the molecular degree of freedom as a point particle, so that the only structure of the molecule arises from its coupling to the atoms. We refer to this model as the *Resonance Model*. The parameters of the Resonance Model can be defined by specifying the S-wave phase shift of the atoms to be

$$k \cot \delta_0(k) = -\frac{8\pi}{m} \left(\lambda - \frac{mg^2}{m\nu - k^2} \right)^{-1}. \quad (115)$$

The three parameters can be interpreted as the detuning energy ν of the molecule relative to the 2-atom threshold, the coupling strength g of the molecule to a pair of atoms, and the self-coupling strength λ of the atoms.

The scattering length and the effective range are

$$a = \frac{m}{8\pi} \left(\lambda - \frac{g^2}{\nu} \right), \quad (116a)$$

$$r_s = -16\pi \left(\lambda - \frac{g^2}{\nu} \right)^{-2} \frac{g^2}{m^2 \nu^2}. \quad (116b)$$

Note that the effective range is negative definite. If $\lambda = 0$, the phase shift in Eq. (115) has the same form as the phase shift for the Effective Range Model in Eq. (60). Thus the Effective Range Model with $r_s < 0$ is a special case of the Resonance Model. The scattering length in Eq. (116a) can be made large by tuning the energy gap ν to near 0. The limiting value of the effective range is $r_s \rightarrow -16\pi/(m^2 g^2)$.

The Resonance Model provides a natural description of atoms near a Feshbach resonance, where the dependence of the scattering length a on the magnetic field B has the form given in Eq. (23). That dependence can be reproduced by taking ν to be linear in the magnetic field B while g^2 and λ are proportional to a_{bg} :

$$\nu = -\mu_i (B - B_i), \quad (117a)$$

$$\lambda = \frac{8\pi a_{\text{bg}}}{m}, \quad (117b)$$

$$g^2 = -\frac{8\pi a_{\text{bg}}}{m} \mu_i \Delta_i. \quad (117c)$$

The parameter μ_i in Eq. (117) can be interpreted as the difference between the magnetic moment of the molecule and twice the magnetic moment of an isolated atom. In general, both a_{bg} and μ_i can be slowly-varying functions of the magnetic field.

The Resonance Model was first introduced by Kaplan as a model for non-relativistic particles with a large scattering length [26]. He used dimensional regularization which eliminated the need for explicit renormalization of the parameters. The Resonance Model was constructed independently by Kokkelmans et al. [27] as a model for atoms near a Feshbach resonance. They derived the renormalization of the parameters that is required to make the observables independent of the ultraviolet momentum cutoff. In Sec. 8.7, we generalize the Resonance Model to one in which the atoms are coupled to N different molecular states.

8.1 Hamiltonian

The Resonance Model can be formulated as a quantum field theory with two complex fields: ψ , which annihilates an atom, and ϕ , which annihilates a di-

atomic molecule. The Hamiltonian density for the Resonance Model is the sum of a free term and an interaction term:

$$\mathcal{H}_{\text{free}} = \frac{1}{2m} \nabla \psi^\dagger \cdot \nabla \psi + \frac{1}{4m} \nabla \phi^\dagger \cdot \nabla \phi + \nu_0 \phi^\dagger \phi, \quad (118a)$$

$$\mathcal{H}_{\text{int}} = \frac{1}{2} g_0 (\phi^\dagger \psi^2 + \psi^{\dagger 2} \phi) + \frac{1}{4} \lambda_0 (\psi^\dagger \psi)^2. \quad (118b)$$

To avoid ultraviolet divergences, an ultraviolet cutoff Λ must be imposed on the momenta of virtual particles.

The Resonance Model is renormalizable in the 2-atom sector, which consists of states containing two atoms or one diatomic molecule. The values for the bare parameters that are required to reproduce the phase shift in Eq. (115) are

$$\lambda_0(\Lambda) = Z(\Lambda) \lambda, \quad (119a)$$

$$g_0(\Lambda) = Z(\Lambda) g, \quad (119b)$$

$$\nu_0(\Lambda) = \nu - [1 - Z(\Lambda)] g^2 / \lambda, \quad (119c)$$

where the renormalization constant Z is

$$Z(\Lambda) = \left(1 - \frac{m}{4\pi^2} \lambda \Lambda \right)^{-1}. \quad (120)$$

Note that in the special case $\lambda = 0$, which corresponds to the Effective Range Model, the only renormalization that is necessary is an additive renormalization of the detuning energy:

$$\nu_0(\Lambda) = \nu + \frac{m}{4\pi^2} g^2 \Lambda. \quad (121)$$

The bare parameter g_0 is equal to its renormalized counterpart g .

Using the renormalizations of the parameters given in Eqs. (119), one can construct two renormalization invariants:

$$g/\lambda = g_0/\lambda_0, \quad (122a)$$

$$\nu - g^2/\lambda = \nu_0 - g_0^2/\lambda_0. \quad (122b)$$

If we take the three independent parameters to be the two renormalization invariants in Eqs. (122) along with λ_0 , the only parameter that must be adjusted as a function of the ultraviolet cutoff is $\lambda_0(\Lambda)$.

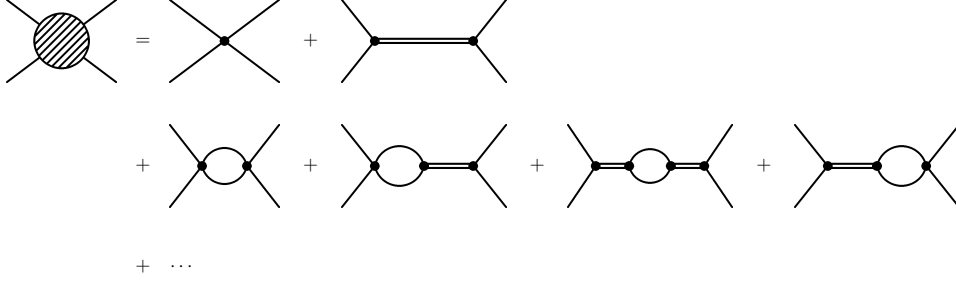


Fig. 5. The series of diagrams that give the amputated connected Green's function for atom-atom scattering in the Resonance Model.

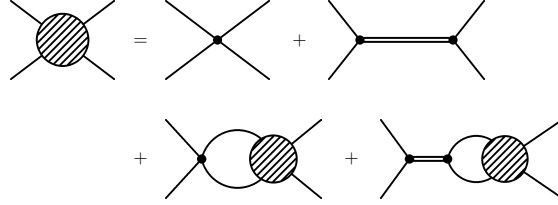


Fig. 6. The integral equation for the amputated connected Green's function for atom-atom scattering in a model with a diatomic molecule that has a coupling to two atoms, such as the Resonance Model.

8.2 Green's function

The amputated connected Green's function for two atoms to evolve into two atoms can be calculated analytically in the Resonance Model by summing the series of diagrams shown in Fig. 5. Alternatively, it can be obtained by solving the integral equation illustrated in Fig. 6. This amplitude depends only on the total energy E of the two atoms in the center-of-mass frame:

$$\mathcal{A}(E) = - \left[\left(\lambda_0 + \frac{g_0^2}{E - \nu_0 + i\varepsilon} \right)^{-1} + \frac{m}{4\pi^2} \Lambda - \frac{m}{8\pi} \kappa \right]^{-1}, \quad (123)$$

where $\kappa = (-mE - i\varepsilon)^{1/2}$. After inserting the renormalization conditions in Eqs. (119), the dependence on the ultraviolet cutoff Λ disappears and the amplitude reduces to

$$\mathcal{A}(E) = - \left[\left(\lambda + \frac{g^2}{E - \nu + i\varepsilon} \right)^{-1} - \frac{m}{8\pi} \kappa \right]^{-1}. \quad (124)$$

8.3 *T-matrix element*

The T-matrix element $\mathcal{T}(k)$ for the scattering of atoms with relative momentum k can be obtained from the amplitude $\mathcal{A}(E)$ in Eq. (124) by setting E equal to the total energy k^2/m of the two atoms:

$$\mathcal{T}(k) = - \left[\left(\lambda - \frac{mg^2}{m\nu - k^2} \right)^{-1} + \frac{i}{8\pi} mk \right]^{-1}. \quad (125)$$

Comparing with Eq. (16), we obtain the S-wave phase shift given in Eq. (115).

8.4 *Bound states*

The amplitude $\mathcal{A}(E)$ in Eq. (124) has poles in the energy variable κ defined by Eq. (52). The values of κ at the poles satisfy

$$\left(\lambda - \frac{mg^2}{m\nu + \kappa^2} \right)^{-1} = \frac{m}{8\pi} \kappa. \quad (126)$$

This can be expressed as a cubic polynomial equation. The number of positive real roots is 0 if $\nu > 0$ and $\lambda < 0$, 1 if ν and λ have the same sign, and 2 if $\nu < 0$ and $\lambda > 0$. Thus the number of stable diatomic molecules can be 0, 1 or 2.

If the scattering length a is made large by tuning ν to near 0, Eq. (126) will have one small root $\kappa \approx 1/a$. If $a > 0$, the corresponding bound state is the shallow dimer. The two remaining roots of Eq. (126) satisfy $|\kappa| \gg 1/|a|$. As $a \rightarrow \pm\infty$, these two large roots approach

$$\kappa_{\pm} \approx \frac{4\pi}{m\lambda} \pm \left[\left(\frac{4\pi}{m\lambda} \right)^2 + \frac{mg^2}{\lambda} \right]^{1/2}. \quad (127)$$

If $\lambda < 0$, neither of these roots is real and positive. If $\lambda > 0$, the root κ_+ is real and positive. It corresponds to a stable deeply-bound diatomic molecule.

8.5 *Optical Theorem*

If the energy E is real, the imaginary part of the amplitude in Eq. (124) is

$$\begin{aligned} \text{Im } \mathcal{A}(E) = & \frac{mk}{8\pi} \left[\left(\lambda - \frac{mg^2}{m\nu - k^2} \right)^{-2} + \left(\frac{mk}{8\pi} \right)^2 \right]^{-1} \theta(E) \\ & + \frac{16\pi^2}{m^2} \sum_i \kappa_i \left[1 + \frac{m^2 g^2 \kappa_i^3}{4\pi(m\nu + \kappa_i^2)^2} \right]^{-1} \delta(E + \kappa_i^2/m) \theta(\kappa_i), \end{aligned} \quad (128)$$

where the sum in the last term is over the 0, 1, or 2 positive real roots κ_i of Eq. (126). The expression for $\text{Im } \mathcal{A}(E)$ in Eq. (128) is positive definite, in accord with the Optical Theorem in Eq. (29). This is consistent with the absence of negative-norm states in the 2-atom sector of the Resonance Model.

8.6 Resonance Model with ghost molecule

The expression in Eq. (116b) for the effective range r_s in the Resonance Model is negative definite. Thus this model cannot be used as a phenomenological description of atoms with positive effective range. Kaplan pointed out that this limitation can be avoided by taking the molecular field ϕ to be a *ghost field* whose quanta are states with negative norm [26]. The Lagrangian for this field theory differs from the Lagrangian for the Resonance Model only in the signs of a few terms. The Lagrangian density is the sum of a free term and an interaction term:

$$\begin{aligned} \mathcal{L}_{\text{free}} = & \psi^\dagger \left(i \frac{\partial}{\partial t} + \frac{\nabla^2}{2m} \right) \psi + \sigma \phi^\dagger \left(i \frac{\partial}{\partial t} + \frac{\nabla^2}{4m} - \sigma \nu_0 \right) \phi, \\ \mathcal{L}_{\text{int}} = & -\frac{1}{2} g_0 (\phi^\dagger \psi^2 + \psi^{\dagger 2} \phi) - \frac{1}{4} \lambda_0 (\psi^\dagger \psi)^2, \end{aligned} \quad (129)$$

where $\sigma = \pm 1$. If $\sigma = +1$, this is the Lagrangian density for the Resonance Model. If $\sigma = -1$, the free theory describes an atom and a ghost molecule. In the Feynman rules for the interacting theory, the only difference from the Resonance Model is in the propagator for the molecule. The propagator for a molecule with energy E and momentum \mathbf{P} is $i/[\sigma(E - P^2/(4m)) - \nu + i\varepsilon]$. The expression for the Green's function in Eq. (124) is replaced by

$$\mathcal{A}(E) = - \left[\left(\lambda + \frac{g^2}{\sigma E - \nu + i\varepsilon} \right)^{-1} - \frac{m}{8\pi} \kappa \right]^{-1}. \quad (130)$$

The S-wave phase shift in Eq. (115) will be modified to

$$k \cot \delta_0(k) = -\frac{8\pi}{m} \left(\lambda - \frac{mg^2}{m\nu - \sigma k^2} \right)^{-1}. \quad (131)$$

The scattering length is given by Eq. (116a) for either sign σ . The effective range differs from the expression in Eq. (116b) by a factor of σ :

$$r_s = -16\pi \sigma \left(\lambda - \frac{g^2}{\nu} \right)^{-2} \frac{g^2}{m^2 \nu^2}. \quad (132)$$

If $\sigma = -1$, this is positive definite.

The amplitude in Eq. (130) has poles in the energy variable κ defined by Eq. (52). The values of κ at the poles are roots of the equation

$$\left(\lambda - \frac{mg^2}{m\nu + \sigma \kappa^2} \right)^{-1} = \frac{m}{8\pi} \kappa. \quad (133)$$

If $\sigma = -1$, the number of positive real roots can be 0 or 2 if ν and λ have the same sign and 1 or 3 if they have opposite signs. If the energy E is real, the imaginary part of the amplitude in Eq. (124) is

$$\begin{aligned} \text{Im } \mathcal{A}(E) = & \frac{mk}{8\pi} \left[\left(\lambda - \frac{mg^2}{m\nu - \sigma k^2} \right)^{-2} + \left(\frac{mk}{8\pi} \right)^2 \right]^{-1} \theta(E) \\ & + \frac{16\pi^2}{m^2} \sum_i \kappa_i \left[1 + \frac{\sigma m^2 g^2 \kappa_i^3}{4\pi(m\nu + \sigma \kappa_i^2)^2} \right]^{-1} \delta(E + \kappa_i^2/m) \theta(\kappa_i), \end{aligned} \quad (134)$$

where the sum in the last term is over the 0, 1, 2, or 3 positive real roots κ_i of Eq. (133). Note that if $\sigma = -1$, the last term need not be positive definite. Thus this model may have states that correspond to diatomic molecules with negative norm.

The scattering length in Eq. (116a) can be made large by tuning the energy gap ν to be near 0. The limiting value of the effective range for $\sigma = -1$ is $r_s \rightarrow 16\pi/(m^2 g^2)$, which is positive. There is one small root of Eq. (133) that approaches $\kappa \approx 1/a$ in this limit. If $a > 0$, the corresponding bound state is the shallow dimer. For this root, the delta function contribution in Eq. (134) has a positive coefficient, so the shallow dimer has positive norm. The two remaining roots of Eq. (133) satisfy $|\kappa| \gg 1/|a|$. As $a \rightarrow \pm\infty$, these two large roots approach

$$\kappa_{\pm} \approx \frac{4\pi}{m\lambda} \pm \left[\left(\frac{4\pi}{m\lambda} \right)^2 + \sigma \frac{mg^2}{\lambda} \right]^{1/2}. \quad (135)$$

For the Resonance Model with a ghost molecule, we set $\sigma = -1$. A root κ that is real and positive corresponds to a stable deeply-bound state. If the

root is in the range $0 < \kappa < m^2 g^2 / (4\pi)$, the delta function contribution in Eq. (134) has a negative coefficient, so the bound state is a negative-norm state. If $\lambda < 0$, the only large positive real root is κ_+ , and it corresponds to a negative-norm deeply-bound bound state. If $0 < \lambda < 16\pi^2 / (m^3 g^2)$, both κ_+ and κ_- are positive real roots. They correspond to a positive-norm and a negative-norm deeply-bound state, respectively. If $\lambda > 16\pi^2 / (m^3 g^2)$, there are no large positive real roots, so there are no stable deeply-bound states. Even if it includes deeply-bound negative-norm states, the Resonance Model with $\sigma = -1$ may still be useful as an approximate description of atoms with a large scattering length and a positive effective range at energies small compared to $1/(mr_s^2)$.

8.7 Multi-resonance models

The *Resonance Model* can be generalized to one with N diatomic molecules that couple to a pair of atoms but not to each other. We refer to this model as the *N-Resonance Model*. It has $2N+1$ parameters: the self-coupling strength λ for the atoms, a detuning energy ν_n for each of the N molecules, and a coupling strength g_n for each of the N molecules. The parameters in the *N-Resonance Model* can be defined by specifying the S-wave phase shift to be

$$k \cot \delta_0(k) = -\frac{8\pi}{m} \left(\lambda - \sum_{n=1}^N \frac{mg_n^2}{m\nu_n - k^2} \right)^{-1}. \quad (136)$$

The scattering length and the effective range are

$$a = \frac{m}{8\pi} \left(\lambda - \sum_{n=1}^N \frac{g_n^2}{\nu_n} \right), \quad (137a)$$

$$r_s = -16\pi \left(\lambda - \sum_{n=1}^N \frac{g_n^2}{\nu_n} \right)^{-2} \sum_{n=1}^N \frac{g_n^2}{m^2 \nu_n^2}. \quad (137b)$$

Note that the effective range is negative definite.

The Hamiltonian density for the *N-Resonance Model* is the sum of a free term and an interaction term:

$$\mathcal{H}_{\text{free}} = \frac{1}{2m} \nabla \psi^\dagger \cdot \nabla \psi + \sum_{n=1}^N \left(\frac{1}{4m} \nabla \phi_n^\dagger \cdot \nabla \phi_n + \nu_{0,n} \phi_n^\dagger \phi_n \right), \quad (138a)$$

$$\mathcal{H}_{\text{int}} = \frac{\lambda_0}{4} (\psi^\dagger \psi)^2 + \sum_{n=1}^N \frac{g_{0,n}}{2} (\phi_n^\dagger \psi^2 + \psi^{\dagger 2} \phi_n). \quad (138b)$$

As we will show below, the relation between the bare coupling constants in Eq. (138) and the renormalized parameters in Eq. (136) can be expressed compactly as an equality between two functions of the energy E :

$$\left(\lambda + \sum_{n=1}^N \frac{g_n^2}{E - \nu_n}\right)^{-1} = \left(\lambda_0 + \sum_{n=1}^N \frac{g_{0,n}^2}{E - \nu_{0,n}}\right)^{-1} + \frac{m}{4\pi^2}\Lambda. \quad (139)$$

By taking the limit $E \rightarrow \infty$, we find that the relation between λ_0 and λ has the same form in Eq. (119a) as in the Resonance Model. Both sides of Eq. (139) can be expressed as ratios of polynomials in E of degree N . The equality between these rational functions can be expressed as $2N$ coupled nonlinear equations for the remaining $2N$ parameters of the N -Resonance Model.

The amputated connected Green's function for two atoms to evolve into two atoms can be calculated analytically by solving the integral equation represented diagrammatically in Fig. 6. The amplitude \mathcal{A} depends only on the total energy E in the center-of-mass frame:

$$\mathcal{A}(E) = - \left[\left(\lambda_0 + \sum_{n=1}^N \frac{g_{0,n}^2}{E - \nu_{0,n} + i\varepsilon} \right)^{-1} + \frac{m}{4\pi^2}\Lambda - \frac{m}{8\pi}\kappa \right]^{-1}, \quad (140)$$

where $\kappa = (-mE - i\varepsilon)^{1/2}$. Inside the square brackets in Eq. (140), the sum of the term raised to the power -1 and the term $(m/4\pi^2)\Lambda$ can be expressed as the ratio of two N th order polynomials in E . By the fundamental theorem of arithmetic, the polynomial in the numerator has N zeroes in the complex plane, which we denote by ν_n , $n = 1, \dots, N$. Except on sets of the bare parameters that have measure zero, those zeroes will be distinct. By decomposing the inverse of that ratio of polynomials into partial fractions, the amplitude in Eq. (140) can be expressed in the form

$$\mathcal{A}(E) = - \left[\left(\lambda + \sum_{n=1}^N \frac{g_n^2}{E - \nu_n + i\varepsilon} \right)^{-1} - \frac{m}{8\pi}\kappa \right]^{-1}. \quad (141)$$

By comparing Eqs. (140) and (141), we obtain the renormalization condition in Eq. (139).

The condition that the Hamiltonian be hermitian requires that the bare parameters λ_0 , $\nu_{0,n}$ and $g_{0,n}$ in the Hamiltonian density in Eqs. (138) be real valued. The expression in Eq. (140) is therefore a real-valued function for real κ . This implies that the parameters ν_n and g_n^2 in Eq. (141) are either real or they come in complex conjugate pairs. This is sufficient to guarantee that the phase shift in Eq. (136) is real valued, which is necessary if the model is to

describe atoms that have no inelastic scattering channels. To show that the N -Resonance Model is renormalizable in the 2-atom sector for arbitrary real values of the parameters ν_n and g_n , one must show that the renormalization conditions in Eq. (139) have real solutions for the bare parameters $\nu_{0,n}$ and $g_{0,n}$ as $\Lambda \rightarrow \infty$. We will verify this below for the Two-Resonance Model. We have not shown that this is the case for the N -Resonance Model with $N \geq 3$.

The renormalization conditions for the Two-Resonance Model are obtained by setting $N = 2$ in Eq. (139). We can use Eq. (120) to express the ultraviolet cutoff Λ as a function of λ and Z :

$$\Lambda = \frac{4\pi^2}{m\lambda} (1 - Z^{-1}). \quad (142)$$

If we also use Eq. (119a) to eliminate λ_0 in favor of λ and Z , the renormalization condition in Eq. (139) reduces to

$$\begin{aligned} & \frac{(E - \nu_1)(E - \nu_2)}{(E - \nu_1)(E - \nu_2) + [g_1^2(E - \nu_2) + g_2^2(E - \nu_1)]/\lambda} \\ &= \frac{(E - \nu_{0,1})(E - \nu_{0,2}) + (Z^{-1} - Z^{-2})[g_{0,1}^2(E - \nu_{0,2}) + g_{0,2}^2(E - \nu_{0,1})]/\lambda}{(E - \nu_{0,1})(E - \nu_{0,2}) + Z^{-1}[g_{0,1}^2(E - \nu_{0,2}) + g_{0,2}^2(E - \nu_{0,1})]/\lambda}. \end{aligned} \quad (143)$$

We obtain four coupled equations by matching the constant terms and the linear terms in E in both the numerator and denominator:

$$\nu_1\nu_2 = \nu_{0,1}\nu_{0,2} - Z^{-1}(1 - Z^{-1})(g_{0,1}^2\nu_{0,2} + g_{0,2}^2\nu_{0,1})/\lambda, \quad (144a)$$

$$\nu_1 + \nu_2 = \nu_{0,1} + \nu_{0,2} - Z^{-1}(1 - Z^{-1})(g_{0,1}^2 + g_{0,2}^2)/\lambda, \quad (144b)$$

$$\nu_1\nu_2 - (g_1^2\nu_2 + g_2^2\nu_1)/\lambda = \nu_{0,1}\nu_{0,2} - Z^{-1}(g_{0,1}^2\nu_{0,2} + g_{0,2}^2\nu_{0,1})/\lambda, \quad (144c)$$

$$\nu_1 + \nu_2 - (g_1^2 + g_2^2)/\lambda = \nu_{0,1} + \nu_{0,2} - Z^{-1}(g_{0,1}^2 + g_{0,2}^2)/\lambda. \quad (144d)$$

These equations can be solved for the bare parameters as functions of the renormalized parameters and Z :

$$\nu_{0,1} = \frac{1}{2} (\bar{\nu}_1 + \bar{\nu}_2 + C), \quad (145a)$$

$$\nu_{0,2} = \frac{1}{2} (\bar{\nu}_1 + \bar{\nu}_2 - C), \quad (145b)$$

$$g_{0,1} = \frac{Z}{\sqrt{2}} \left(g_1^2 + g_2^2 + \frac{D}{C} \right)^{1/2}, \quad (145c)$$

$$g_{0,2} = \frac{Z}{\sqrt{2}} \left(g_1^2 + g_2^2 - \frac{D}{C} \right)^{1/2}, \quad (145d)$$

where

$$\bar{\nu}_1 = \nu_1 - (1 - Z) g_1^2 / \lambda, \quad (146a)$$

$$\bar{\nu}_2 = \nu_2 - (1 - Z) g_2^2 / \lambda, \quad (146b)$$

$$C = \left[(\bar{\nu}_1 - \bar{\nu}_2)^2 + 4(1 - Z)^2 g_1^2 g_2^2 / \lambda^2 \right]^{1/2}, \quad (146c)$$

$$D = (\bar{\nu}_1 - \bar{\nu}_2)(g_1^2 - g_2^2) - 4(1 - Z) g_1^2 g_2^2 / \lambda. \quad (146d)$$

Note that the expressions for the bare parameters $\nu_{0,1}$, $g_{0,1}$, $\nu_{0,2}$, and $g_{0,2}$ in Eq. (145) are each separately symmetric under the interchange of the renormalized parameters: $\nu_1 \leftrightarrow \nu_2$ and $g_1 \leftrightarrow g_2$. The Two-Resonance Model is renormalizable for given values of ν_1 , g_1 , ν_2 , and g_2 if the solutions for the bare parameters in Eq. (145) are real valued in the limit $\Lambda \rightarrow \infty$. Since the expression for C in Eq. (146c) is the square root of a manifestly positive quantity, it is clear that the parameters $\nu_{0,1}$ and $\nu_{0,2}$ in Eqs. (145a) and (145b) are real. The condition that the parameters $g_{0,1}$ and $g_{0,2}$ in Eqs. (145c) and (145d) are real is $g_1^2 + g_2^2 > |D|/C$. It is easy to verify that this is satisfied for any real values of ν_1 , ν_2 , g_1 , and g_2 , even at finite Λ .

The Two-Resonance Model has been previously discussed in Ref. [27], but their results for the renormalization of the parameters of the model are incorrect. They obtained the correct result in Eq. (119a) for the renormalization of λ . However, their results for the renormalizations of the parameters ν_1 and g_1 for the first resonance are given by the same simple equations in Eqs. (119b) and (119c) as in the Resonance Model, while their results for the renormalizations of the parameters ν_2 and g_2 for the second resonance are given by more complicated equations. It is easy to see from symmetry considerations that these results cannot be correct. The Hamiltonian of the N -Resonance Model is symmetric under the interchange $\phi_1 \leftrightarrow \phi_2$ of the two molecular fields if we also interchange the bare parameters: $\nu_{0,1} \leftrightarrow \nu_{0,2}$ and $g_{0,1} \leftrightarrow g_{0,2}$. Thus the expressions for the bare parameters $\nu_{1,0}$ and $g_{1,0}$ should differ from those for $\nu_{2,0}$ and $g_{2,0}$ simply by interchange of the renormalized parameters. Our expressions for the renormalized parameters in Eqs. (145) satisfy this condition, but those in Ref. [27] do not.

The amplitude in Eq. (141) has poles in the energy variable κ defined by Eq. (52). The values of κ at the poles are roots of the equation

$$\left(\lambda - \sum_{n=1}^N \frac{m g_n^2}{m \nu_n + \kappa^2} \right)^{-1} = \frac{m}{8\pi} \kappa. \quad (147)$$

If the energy E is real, the imaginary part of the amplitude in Eq. (141) is

$$\begin{aligned} \text{Im } \mathcal{A}(E) = & \frac{mk}{8\pi} \left[\left(\lambda - \sum_{n=1}^N \frac{mg_n^2}{m\nu_n - k^2} \right)^{-2} + \left(\frac{mk}{8\pi} \right)^2 \right]^{-1} \theta(E) \\ & + \frac{16\pi^2}{m^2} \sum_i \kappa_i \left[1 + \sum_{n=1}^N \frac{m^2 g_n^2 \kappa_i^3}{4\pi(m\nu_n + \kappa_i^2)^2} \right]^{-1} \delta(E + \kappa_i^2/m) \theta(\kappa_i), \end{aligned} \quad (148)$$

where the sum in the last term is over the positive real roots κ_i of Eq. (147). This expression is positive definite, in accord with the Optical Theorem in Eq. (29). This is consistent with the absence of negative-norm states in the 2-atom sector of the N -Resonance Model.

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A Integrals

Some of the results in this paper require the evaluation of integrals over the momentum \mathbf{k} of virtual atoms of the form

$$I_{2n}(E) = \int \frac{d^3k}{(2\pi)^3} \frac{k^{2n}}{E - k^2/m + i\varepsilon}, \quad (\text{A.1})$$

where n is an integer. These integrals are functions of the total energy E of a pair of atoms in the center-of-mass frame. It is convenient to express them in terms of the variable $\kappa = (-mE - i\varepsilon)^{1/2}$ defined in Eq. (52). For $n \geq 0$, the integrals given by Eq. (A.1) are ultraviolet divergent. They can be regularized by imposing a momentum cutoff: $|\mathbf{k}| < \Lambda$. The integrals then satisfy a simple recursion relation:

$$I_{2n}(E) = -\frac{m}{2\pi^2} \frac{\Lambda^{2n+1}}{2n+1} - \kappa^2 I_{2n-2}(E). \quad (\text{A.2})$$

This can be used to express the integrals $I_{2n}(E)$ for $n \geq 1$ in terms of $I_0(E)$, whose value is

$$I_0(E) = -\frac{m}{2\pi^2} \left(\Lambda - \kappa \arctan \frac{\Lambda}{\kappa} \right). \quad (\text{A.3})$$

The expressions for the integrals are particularly simple if we take Λ to be so much larger than $(m|E|)^{1/2}$ that we can neglect terms that decrease as inverse powers of $\Lambda/(m|E|)^{1/2}$ as $\Lambda \rightarrow \infty$. The integral in Eq. (A.3) then reduces to

$$I_0(E) = -\frac{m}{2\pi^2} \left(\Lambda - \frac{\pi}{2} \kappa \right). \quad (\text{A.4})$$

The next two integrals in the sequence are

$$I_2(E) = -\frac{m}{2\pi^2} \left(\frac{1}{3} \Lambda^3 - \Lambda \kappa^2 + \frac{\pi}{2} \kappa^3 \right), \quad (\text{A.5a})$$

$$I_4(E) = -\frac{m}{2\pi^2} \left(\frac{1}{5} \Lambda^5 - \frac{1}{3} \Lambda^3 \kappa^2 + \Lambda \kappa^4 - \frac{\pi}{2} \kappa^5 \right). \quad (\text{A.5b})$$

With dimensional regularization, the integral in Eq. (A.1) is generalized to an integral over a space with dimension $3 - 2\epsilon$ and then analytically continued to $\epsilon = 0$. This procedure automatically subtracts any power ultraviolet divergences. The resulting expressions for the integrals can be obtained simply by setting $\Lambda = 0$ in Eqs. (A.4) and (A.5):

$$I_0(E) = \frac{m}{4\pi} \kappa, \quad (\text{A.6a})$$

$$I_2(E) = -\frac{m}{4\pi} \kappa^3, \quad (\text{A.6b})$$

$$I_4(E) = \frac{m}{4\pi} \kappa^5. \quad (\text{A.6c})$$

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